



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 30, 2026 – 01:26 AM UTC

PDB ID : 6YJ0 / pdb\_00006yj0  
BMRB ID : 50015  
Title : Solution NMR structure of titin N2A region Ig domain I83  
Authors : Pfuhl, M.; Gage, M.  
Deposited on : 2020-04-02

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
BMRB Restraints Analysis : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

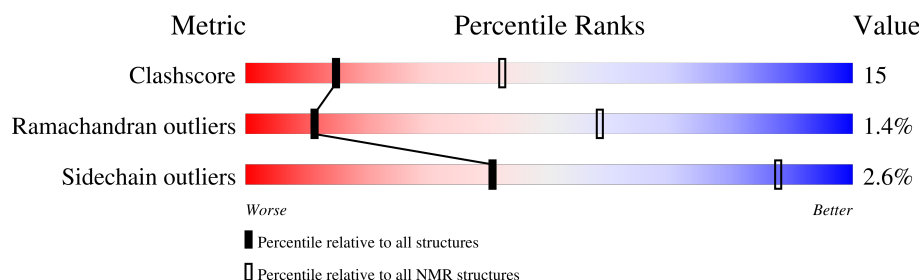
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 92%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | NMR archive<br>(#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore            | 229148                      | 14424                     |
| Ramachandran outliers | 224038                      | 12848                     |
| Sidechain outliers    | 223484                      | 12823                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 105    |                  |

## 2 Ensemble composition and analysis

This entry contains 40 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

| Well-defined (core) protein residues |                            |                   |              |
|--------------------------------------|----------------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total)      | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:11-A:83, A:91-A:100 (83) | 0.14              | 14           |

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 7 clusters and 3 single-model clusters were found.

| Cluster number        | Models                                                        |
|-----------------------|---------------------------------------------------------------|
| 1                     | 1, 11, 14, 18, 20, 21, 22, 23, 25, 29, 30, 32, 35, 36, 37, 39 |
| 2                     | 3, 8, 10, 12, 13, 16, 19, 26, 33, 40                          |
| 3                     | 27, 31, 38                                                    |
| 4                     | 2, 24                                                         |
| 5                     | 5, 17                                                         |
| 6                     | 4, 9                                                          |
| 7                     | 6, 7                                                          |
| Single-model clusters | 15; 28; 34                                                    |

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1632 atoms, of which 795 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Titin.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 105      | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1632  | 520 | 795 | 145 | 168 | 4 |       |

There are 14 discrepancies between the modelled and reference sequences:

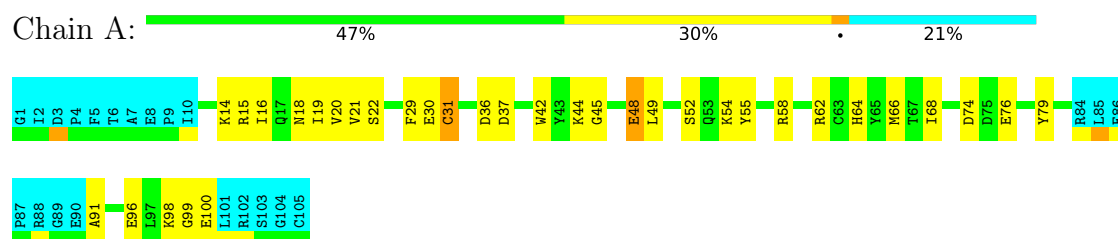
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 1       | GLY      | -      | expression tag | UNP A2ASS6 |
| A     | 2       | ILE      | -      | expression tag | UNP A2ASS6 |
| A     | 3       | ASP      | -      | expression tag | UNP A2ASS6 |
| A     | 4       | PRO      | -      | expression tag | UNP A2ASS6 |
| A     | 5       | PHE      | -      | expression tag | UNP A2ASS6 |
| A     | 6       | THR      | -      | expression tag | UNP A2ASS6 |
| A     | 98      | LYS      | -      | expression tag | UNP A2ASS6 |
| A     | 99      | GLY      | -      | expression tag | UNP A2ASS6 |
| A     | 100     | GLU      | -      | expression tag | UNP A2ASS6 |
| A     | 101     | LEU      | -      | expression tag | UNP A2ASS6 |
| A     | 102     | ARG      | -      | expression tag | UNP A2ASS6 |
| A     | 103     | SER      | -      | expression tag | UNP A2ASS6 |
| A     | 104     | GLY      | -      | expression tag | UNP A2ASS6 |
| A     | 105     | CYS      | -      | expression tag | UNP A2ASS6 |

## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Titin

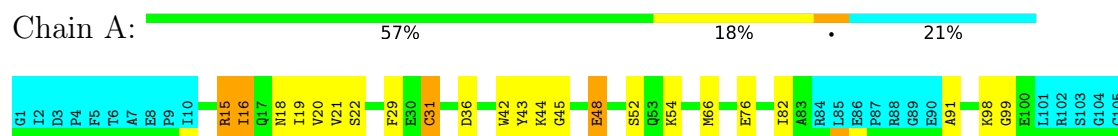


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

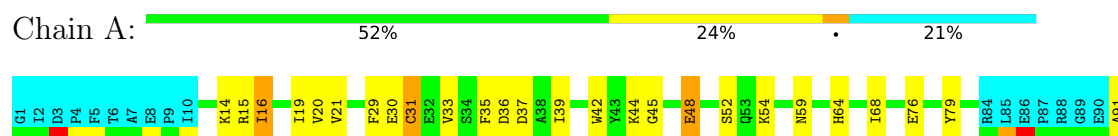
#### 4.2.1 Score per residue for model 1

- Molecule 1: Titin



#### 4.2.2 Score per residue for model 2

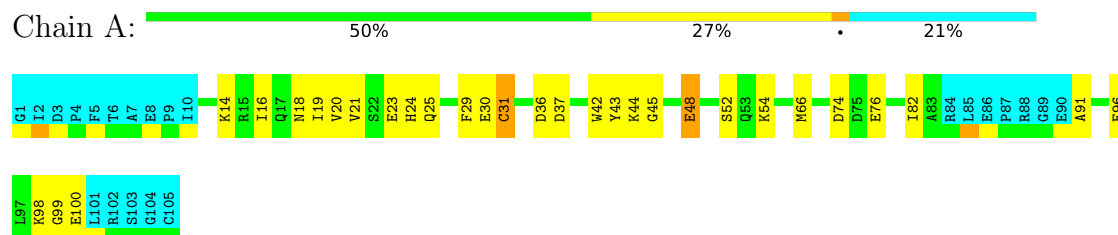
- Molecule 1: Titin





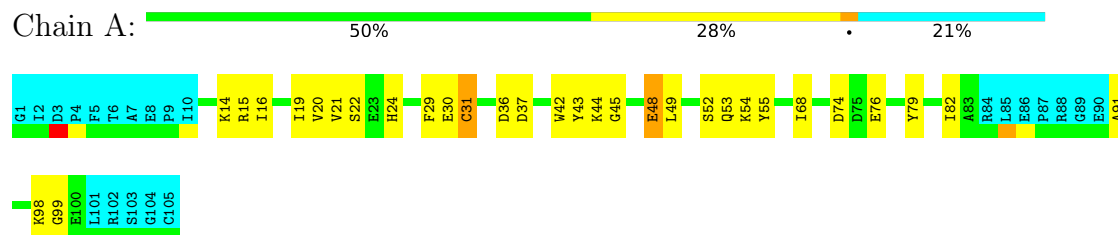
### 4.2.3 Score per residue for model 3

- Molecule 1: Titin



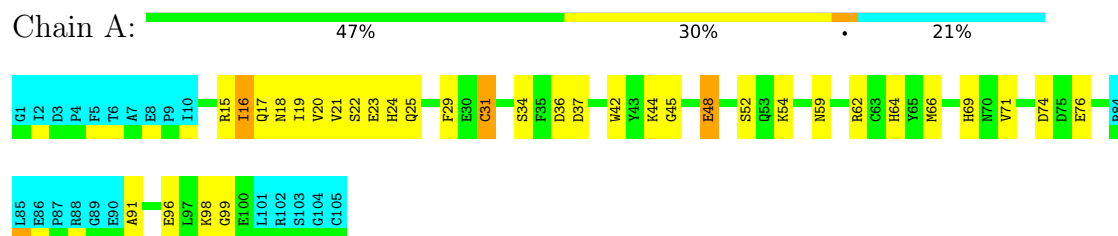
### 4.2.4 Score per residue for model 4

- Molecule 1: Titin



### 4.2.5 Score per residue for model 5

- Molecule 1: Titin



### 4.2.6 Score per residue for model 6

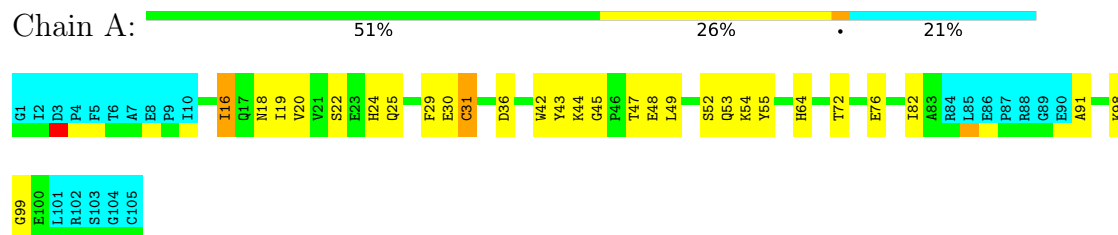
- Molecule 1: Titin





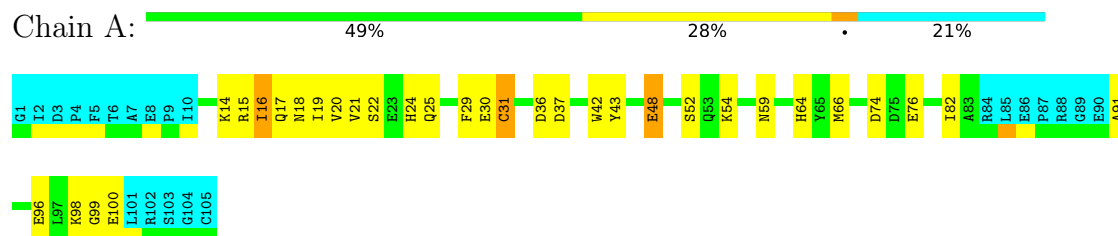
#### 4.2.7 Score per residue for model 7

- Molecule 1: Titin



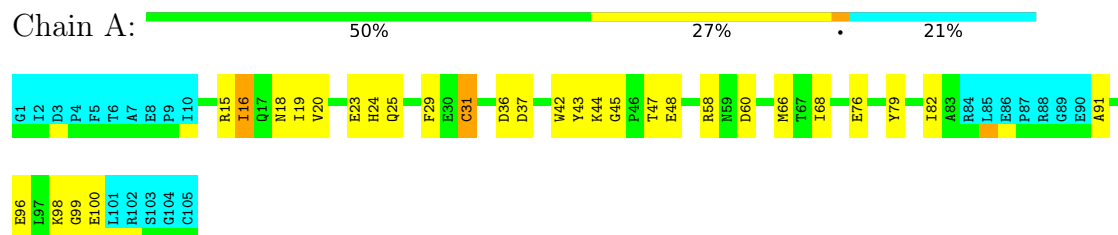
#### 4.2.8 Score per residue for model 8

- Molecule 1: Titin



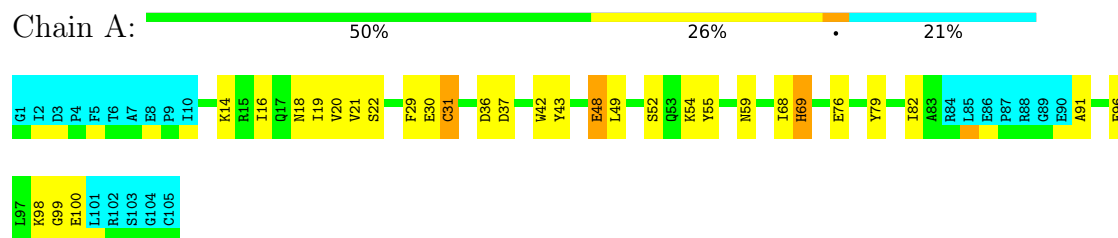
#### 4.2.9 Score per residue for model 9

- Molecule 1: Titin



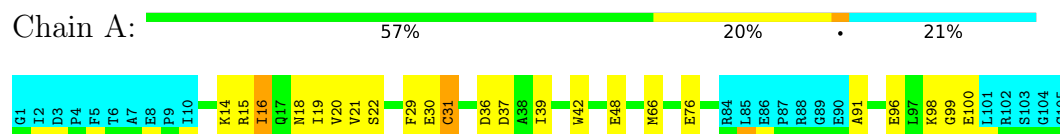
#### 4.2.10 Score per residue for model 10

- Molecule 1: Titin



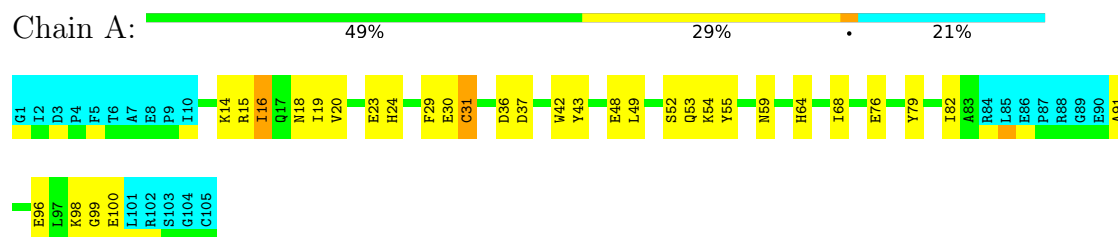
#### 4.2.11 Score per residue for model 11

- Molecule 1: Titin



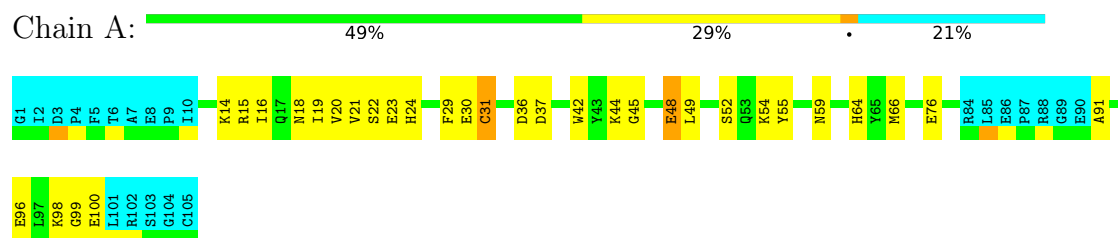
#### 4.2.12 Score per residue for model 12

- Molecule 1: Titin



#### 4.2.13 Score per residue for model 13

- Molecule 1: Titin

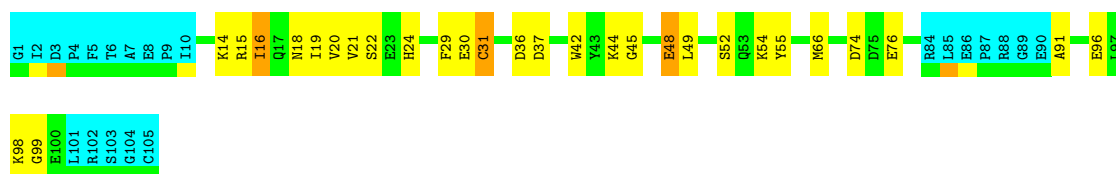


#### 4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: Titin



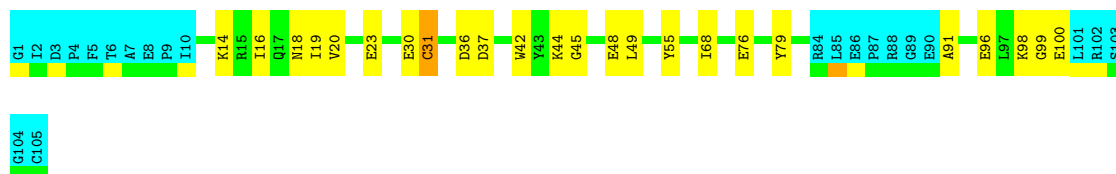




#### 4.2.15 Score per residue for model 15

- Molecule 1: Titin

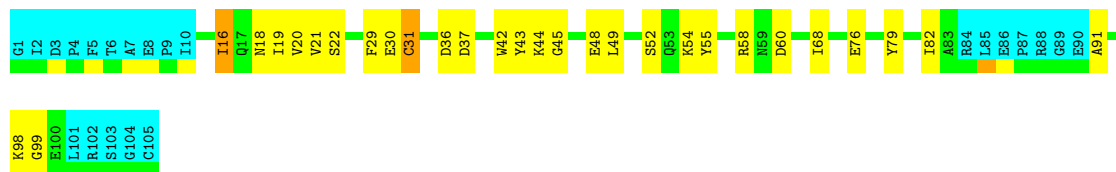
Chain A: 56% 22% 21%



#### 4.2.16 Score per residue for model 16

- Molecule 1: Titin

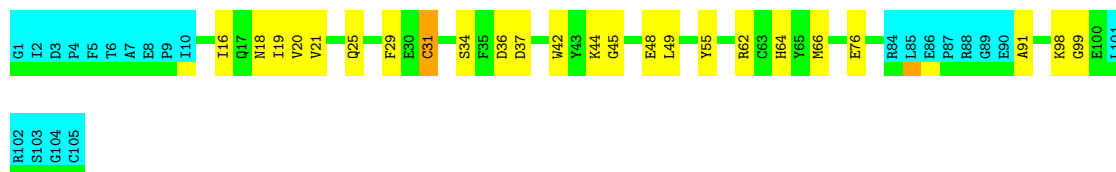
Chain A: 51% 26% 21%



#### 4.2.17 Score per residue for model 17

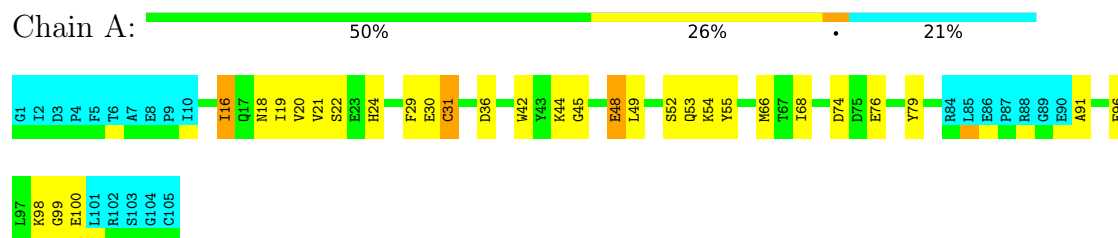
- Molecule 1: Titin

Chain A: 56% 22% 21%



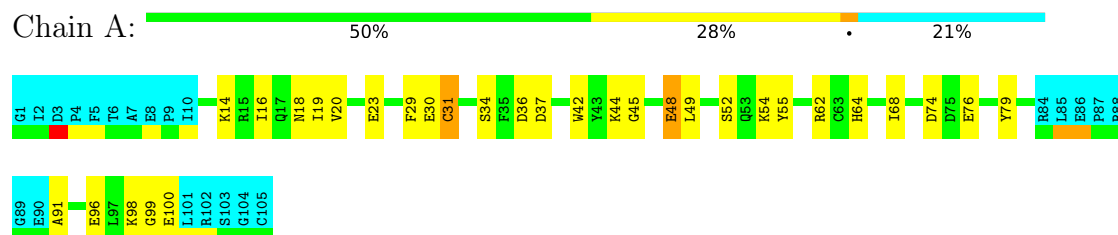
#### 4.2.18 Score per residue for model 18

- Molecule 1: Titin



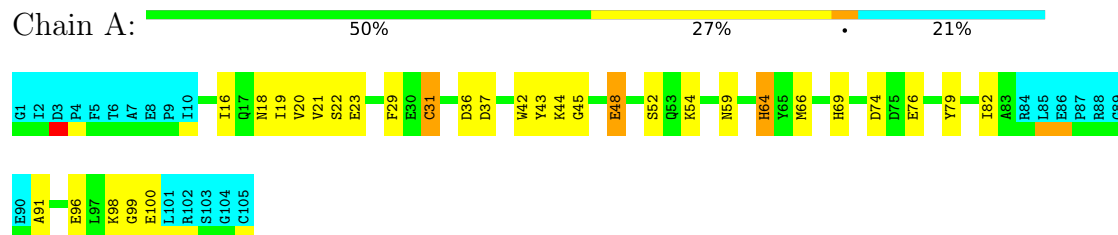
#### 4.2.19 Score per residue for model 19

- Molecule 1: Titin



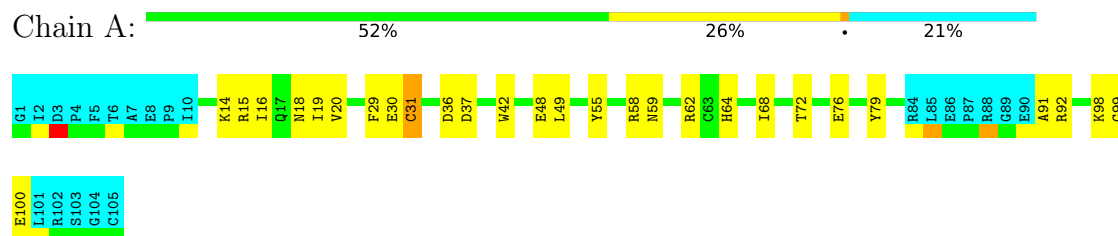
#### 4.2.20 Score per residue for model 20

- Molecule 1: Titin



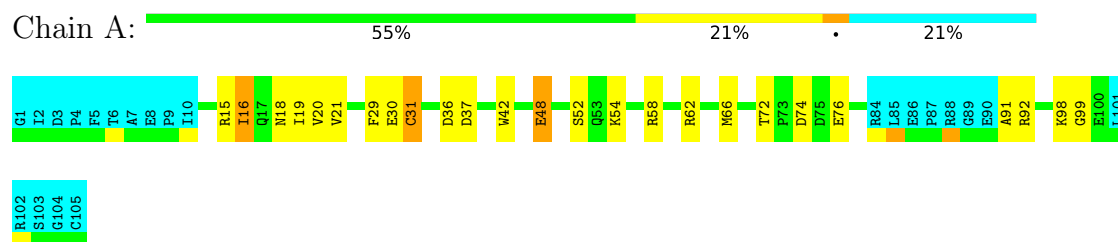
#### 4.2.21 Score per residue for model 21

- Molecule 1: Titin



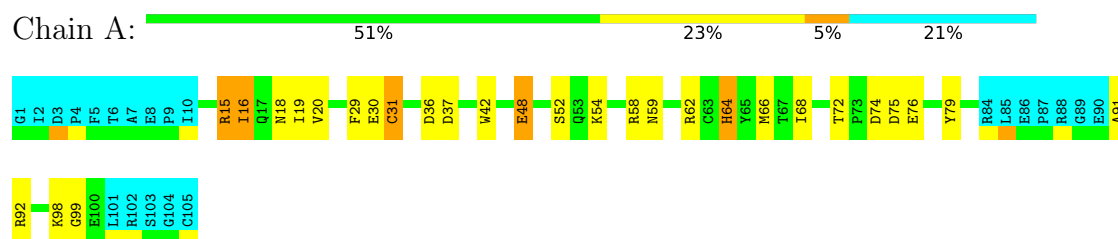
### 4.2.22 Score per residue for model 22

#### • Molecule 1: Titin



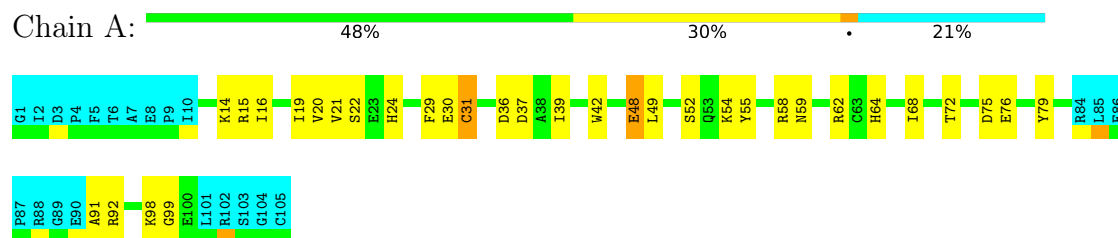
### 4.2.23 Score per residue for model 23

#### • Molecule 1: Titin



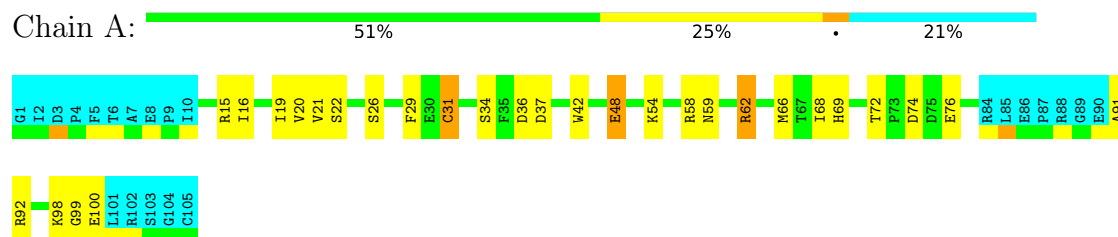
### 4.2.24 Score per residue for model 24

#### • Molecule 1: Titin



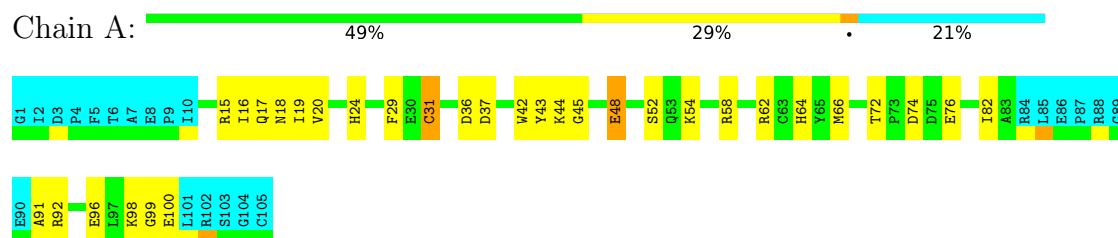
### 4.2.25 Score per residue for model 25

#### • Molecule 1: Titin



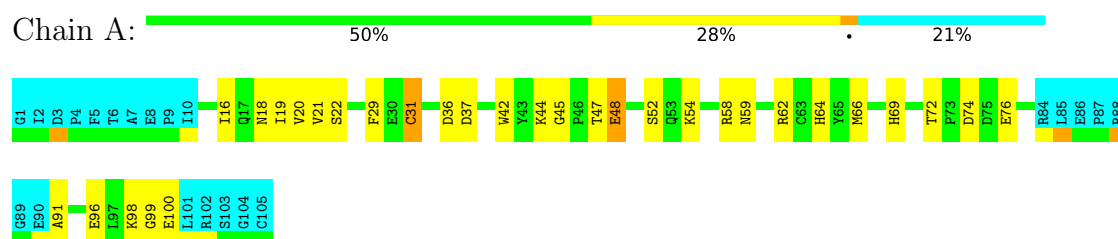
### 4.2.26 Score per residue for model 26

- Molecule 1: Titin



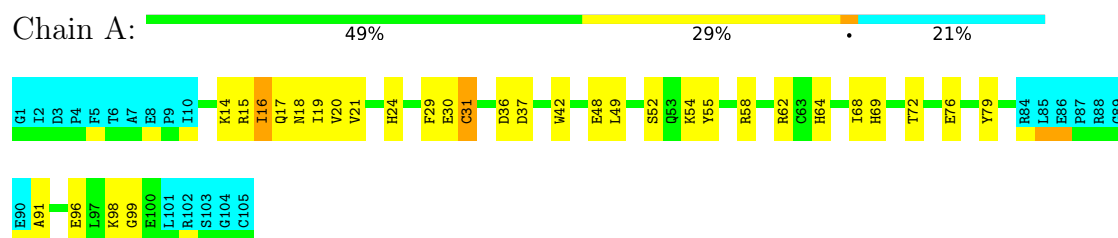
### 4.2.27 Score per residue for model 27

- Molecule 1: Titin



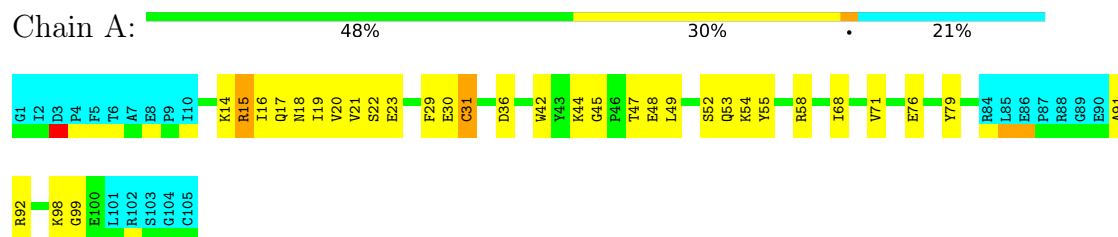
### 4.2.28 Score per residue for model 28

- Molecule 1: Titin



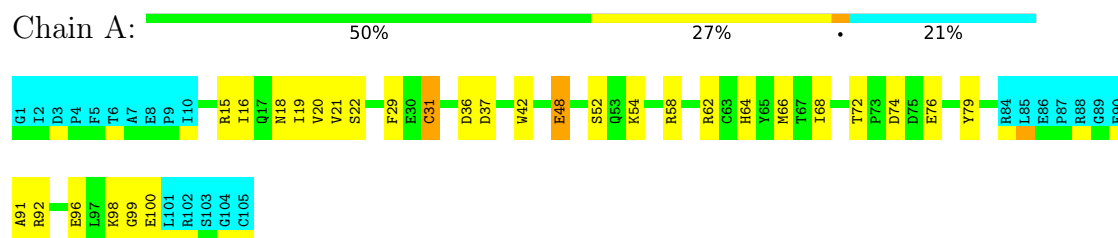
### 4.2.29 Score per residue for model 29

- Molecule 1: Titin



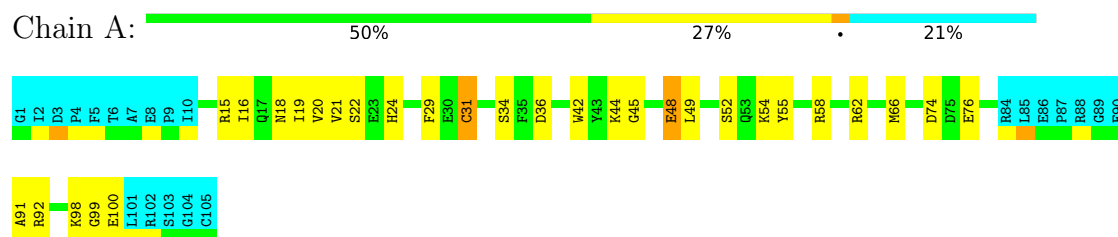
### 4.2.30 Score per residue for model 30

- Molecule 1: Titin



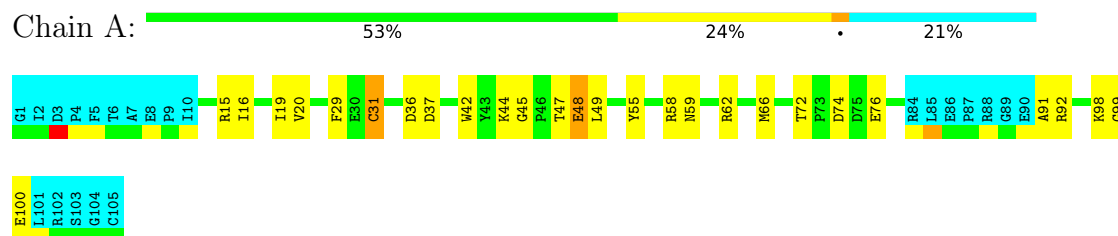
### 4.2.31 Score per residue for model 31

- Molecule 1: Titin



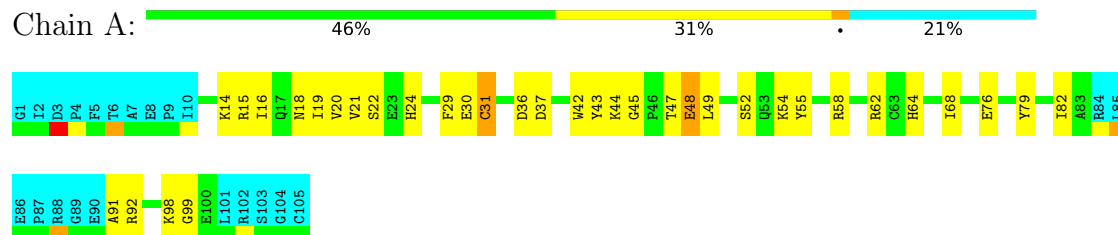
### 4.2.32 Score per residue for model 32

- Molecule 1: Titin



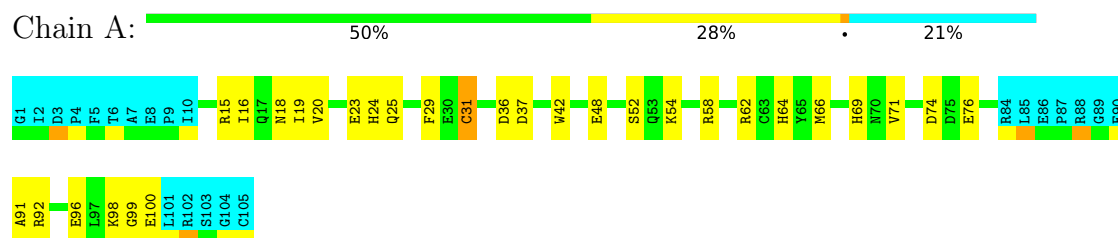
### 4.2.33 Score per residue for model 33

- Molecule 1: Titin



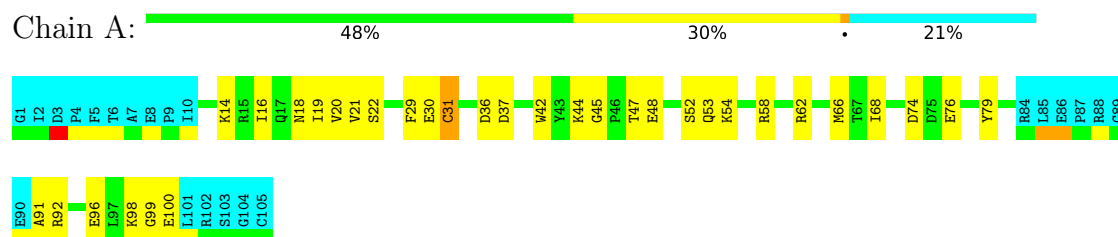
### 4.2.34 Score per residue for model 34

#### • Molecule 1: Titin



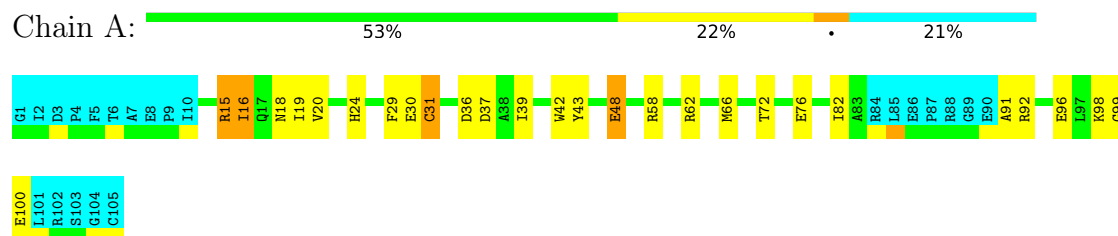
### 4.2.35 Score per residue for model 35

#### • Molecule 1: Titin



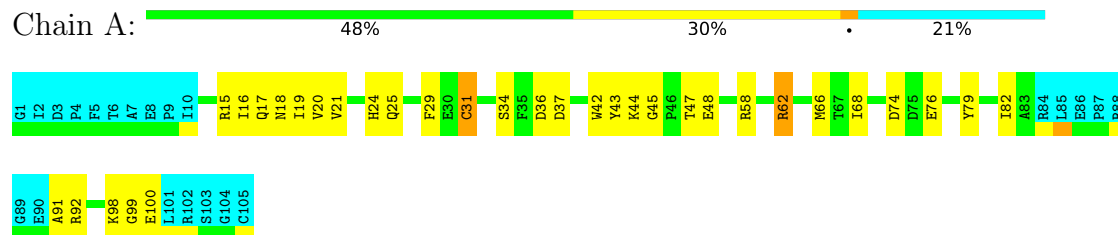
### 4.2.36 Score per residue for model 36

#### • Molecule 1: Titin



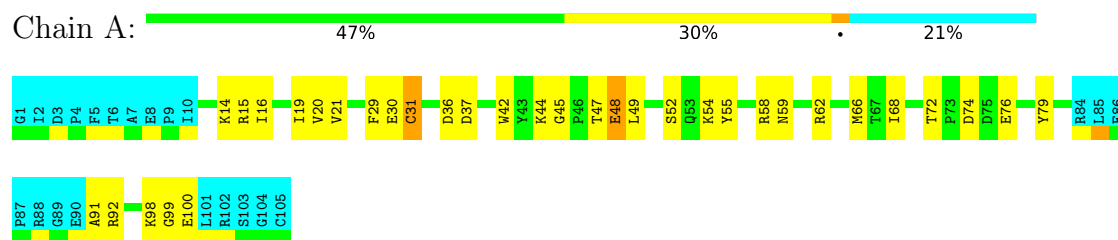
### 4.2.37 Score per residue for model 37

#### • Molecule 1: Titin



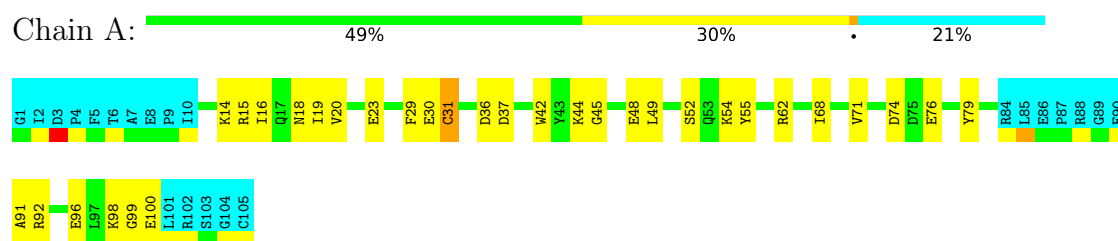
### 4.2.38 Score per residue for model 38

#### • Molecule 1: Titin



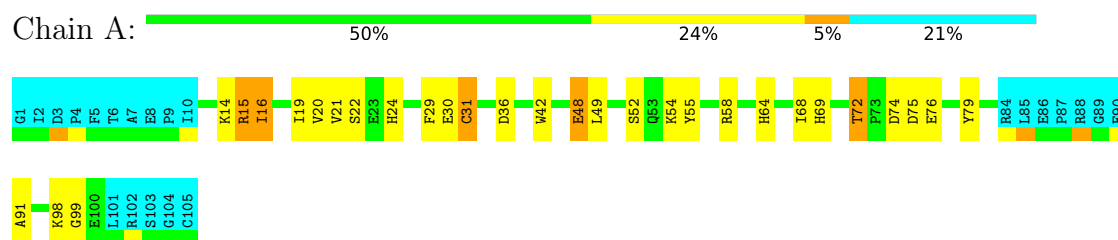
### 4.2.39 Score per residue for model 39

#### • Molecule 1: Titin



### 4.2.40 Score per residue for model 40

#### • Molecule 1: Titin



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 400 calculated structures, 40 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| ARIA          | structure calculation | 2.3.2   |
| X-PLOR NIH    | structure calculation | 2.35    |

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

| Chemical shift file(s)                       | working_cs.cif |
|----------------------------------------------|----------------|
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 1270           |
| Number of shifts mapped to atoms             | 1270           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 92%            |



## 6 Model quality

### 6.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |                      | Bond angles |                      |
|-----|-------|--------------|----------------------|-------------|----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                 |
| 1   | A     | 0.72±0.01    | 0±0/683 ( 0.0± 0.0%) | 1.13±0.01   | 1±1/927 ( 0.1± 0.1%) |
| All | All   | 0.72         | 0/27320 ( 0.0%)      | 1.13        | 23/37080 ( 0.1%)     |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.0±0.0   | 1.8±1.9   |
| All | All   | 0         | 71        |

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|----------|-------|-------------|----------|--------|-------|
|     |       |     |      |          |       |             |          | Worst  | Total |
| 1   | A     | 64  | HIS  | CA-CB-CG | -5.50 | 108.30      | 113.80   | 20     | 12    |
| 1   | A     | 69  | HIS  | CA-CB-CG | -5.49 | 108.31      | 113.80   | 20     | 5     |
| 1   | A     | 53  | GLN  | N-CA-C   | -5.47 | 106.19      | 112.86   | 4      | 6     |

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 58  | ARG  | Sidechain | 19             |
| 1   | A     | 62  | ARG  | Sidechain | 18             |
| 1   | A     | 15  | ARG  | Sidechain | 17             |
| 1   | A     | 92  | ARG  | Sidechain | 17             |

## 6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 668   | 627      | 627      | 20±3    |
| All | All   | 26720 | 25080    | 25080    | 783     |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All unique clashes are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:48:GLU:H    | 1:A:48:GLU:CD   | 0.67     | 1.97        | 1      | 40    |
| 1:A:42:TRP:CG   | 1:A:66:MET:SD   | 0.64     | 2.90        | 31     | 24    |
| 1:A:14:LYS:HZ3  | 1:A:30:GLU:CD   | 0.64     | 2.01        | 15     | 19    |
| 1:A:24:HIS:CE1  | 1:A:25:GLN:HE21 | 0.63     | 2.12        | 3      | 1     |
| 1:A:39:ILE:HD12 | 1:A:39:ILE:N    | 0.61     | 2.10        | 11     | 4     |
| 1:A:43:TYR:CE1  | 1:A:82:ILE:HD12 | 0.60     | 2.31        | 26     | 12    |
| 1:A:24:HIS:CD2  | 1:A:25:GLN:HE21 | 0.60     | 2.14        | 37     | 4     |
| 1:A:16:ILE:HG22 | 1:A:30:GLU:O    | 0.58     | 1.99        | 28     | 7     |
| 1:A:42:TRP:CB   | 1:A:66:MET:SD   | 0.57     | 2.92        | 13     | 24    |
| 1:A:17:GLN:CD   | 1:A:17:GLN:N    | 0.57     | 2.62        | 8      | 1     |
| 1:A:14:LYS:NZ   | 1:A:30:GLU:CD   | 0.57     | 2.63        | 15     | 20    |
| 1:A:76:GLU:OE1  | 1:A:99:GLY:N    | 0.57     | 2.37        | 6      | 21    |
| 1:A:39:ILE:N    | 1:A:39:ILE:CD1  | 0.56     | 2.68        | 36     | 4     |
| 1:A:76:GLU:OE2  | 1:A:99:GLY:N    | 0.56     | 2.38        | 31     | 19    |
| 1:A:18:ASN:OD1  | 1:A:19:ILE:N    | 0.56     | 2.38        | 20     | 10    |
| 1:A:36:ASP:OD2  | 1:A:37:ASP:N    | 0.54     | 2.41        | 36     | 12    |
| 1:A:20:VAL:HG22 | 1:A:98:LYS:HB2  | 0.54     | 1.78        | 21     | 40    |
| 1:A:36:ASP:OD1  | 1:A:37:ASP:N    | 0.53     | 2.41        | 8      | 22    |
| 1:A:54:LYS:NZ   | 1:A:69:HIS:O    | 0.53     | 2.39        | 34     | 4     |
| 1:A:24:HIS:O    | 1:A:24:HIS:CG   | 0.53     | 2.61        | 7      | 6     |
| 1:A:34:SER:O    | 1:A:62:ARG:NH2  | 0.53     | 2.41        | 17     | 5     |
| 1:A:34:SER:O    | 1:A:62:ARG:NH1  | 0.53     | 2.41        | 37     | 1     |
| 1:A:19:ILE:HD12 | 1:A:29:PHE:CE1  | 0.52     | 2.39        | 20     | 18    |
| 1:A:52:SER:C    | 1:A:54:LYS:N    | 0.52     | 2.65        | 19     | 31    |
| 1:A:18:ASN:OD1  | 1:A:96:GLU:O    | 0.52     | 2.28        | 19     | 11    |
| 1:A:14:LYS:HZ2  | 1:A:30:GLU:CD   | 0.52     | 2.13        | 11     | 1     |
| 1:A:31:CYS:SG   | 1:A:42:TRP:CZ2  | 0.52     | 3.03        | 26     | 40    |

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| Atom-1          | Atom-2         | Clash(Å) | Distance(Å) | Models |       |
|-----------------|----------------|----------|-------------|--------|-------|
|                 |                |          |             | Worst  | Total |
| 1:A:31:CYS:SG   | 1:A:42:TRP:CH2 | 0.52     | 3.03        | 26     | 40    |
| 1:A:48:GLU:CD   | 1:A:48:GLU:N   | 0.52     | 2.68        | 20     | 40    |
| 1:A:37:ASP:O    | 1:A:37:ASP:OD2 | 0.51     | 2.28        | 22     | 6     |
| 1:A:19:ILE:HD12 | 1:A:29:PHE:CE2 | 0.51     | 2.40        | 8      | 21    |
| 1:A:37:ASP:O    | 1:A:37:ASP:OD1 | 0.51     | 2.29        | 13     | 3     |
| 1:A:49:LEU:HD22 | 1:A:55:TYR:CZ  | 0.50     | 2.42        | 15     | 19    |
| 1:A:36:ASP:OD1  | 1:A:36:ASP:N   | 0.50     | 2.45        | 1      | 5     |
| 1:A:44:LYS:O    | 1:A:45:GLY:C   | 0.49     | 2.55        | 37     | 26    |
| 1:A:17:GLN:CG   | 1:A:18:ASN:N   | 0.49     | 2.75        | 26     | 5     |
| 1:A:36:ASP:O    | 1:A:36:ASP:OD1 | 0.49     | 2.31        | 7      | 1     |
| 1:A:36:ASP:OD2  | 1:A:36:ASP:N   | 0.48     | 2.44        | 18     | 10    |
| 1:A:18:ASN:O    | 1:A:18:ASN:OD1 | 0.48     | 2.32        | 7      | 6     |
| 1:A:68:ILE:HD11 | 1:A:79:TYR:CE1 | 0.47     | 2.44        | 21     | 10    |
| 1:A:23:GLU:OE1  | 1:A:23:GLU:N   | 0.47     | 2.42        | 3      | 1     |
| 1:A:59:ASN:CG   | 1:A:64:HIS:HD1 | 0.47     | 2.17        | 21     | 9     |
| 1:A:26:SER:OG   | 1:A:68:ILE:O   | 0.47     | 2.31        | 25     | 1     |
| 1:A:59:ASN:O    | 1:A:59:ASN:OD1 | 0.47     | 2.33        | 27     | 6     |
| 1:A:36:ASP:O    | 1:A:36:ASP:OD2 | 0.47     | 2.33        | 31     | 1     |
| 1:A:14:LYS:HZ3  | 1:A:30:GLU:CG  | 0.46     | 2.24        | 39     | 11    |
| 1:A:68:ILE:HD11 | 1:A:79:TYR:CE2 | 0.46     | 2.45        | 24     | 12    |
| 1:A:17:GLN:HG2  | 1:A:18:ASN:N   | 0.46     | 2.26        | 26     | 5     |
| 1:A:23:GLU:O    | 1:A:71:VAL:O   | 0.46     | 2.34        | 39     | 4     |
| 1:A:18:ASN:OD1  | 1:A:96:GLU:N   | 0.46     | 2.47        | 39     | 10    |
| 1:A:74:ASP:O    | 1:A:74:ASP:OD1 | 0.45     | 2.35        | 18     | 5     |
| 1:A:21:VAL:HG12 | 1:A:22:SER:O   | 0.45     | 2.12        | 10     | 20    |
| 1:A:44:LYS:O    | 1:A:47:THR:O   | 0.45     | 2.35        | 37     | 9     |
| 1:A:22:SER:OG   | 1:A:25:GLN:CG  | 0.44     | 2.65        | 7      | 2     |
| 1:A:58:ARG:NE   | 1:A:60:ASP:OD2 | 0.44     | 2.50        | 16     | 1     |
| 1:A:58:ARG:CZ   | 1:A:60:ASP:OD2 | 0.44     | 2.65        | 16     | 1     |
| 1:A:24:HIS:O    | 1:A:24:HIS:ND1 | 0.44     | 2.51        | 28     | 3     |
| 1:A:44:LYS:NZ   | 1:A:79:TYR:CE1 | 0.44     | 2.84        | 20     | 1     |
| 1:A:18:ASN:ND2  | 1:A:18:ASN:N   | 0.44     | 2.64        | 17     | 3     |
| 1:A:76:GLU:CD   | 1:A:99:GLY:H   | 0.44     | 2.20        | 18     | 2     |
| 1:A:68:ILE:CD1  | 1:A:79:TYR:CE1 | 0.43     | 3.01        | 15     | 6     |
| 1:A:74:ASP:OD1  | 1:A:74:ASP:C   | 0.43     | 2.61        | 20     | 4     |
| 1:A:49:LEU:HD22 | 1:A:55:TYR:CE2 | 0.43     | 2.48        | 31     | 3     |
| 1:A:72:THR:OG1  | 1:A:75:ASP:CG  | 0.43     | 2.61        | 24     | 3     |
| 1:A:33:VAL:HG23 | 1:A:35:PHE:O   | 0.43     | 2.14        | 2      | 1     |
| 1:A:74:ASP:OD2  | 1:A:74:ASP:C   | 0.43     | 2.62        | 4      | 4     |
| 1:A:74:ASP:O    | 1:A:74:ASP:OD2 | 0.43     | 2.37        | 30     | 9     |
| 1:A:74:ASP:OD2  | 1:A:74:ASP:O   | 0.42     | 2.37        | 4      | 7     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:59:ASN:O    | 1:A:59:ASN:CG   | 0.42     | 2.63        | 27     | 2     |
| 1:A:15:ARG:O    | 1:A:16:ILE:C    | 0.42     | 2.63        | 8      | 12    |
| 1:A:19:ILE:HG22 | 1:A:21:VAL:HG23 | 0.41     | 1.92        | 14     | 18    |
| 1:A:43:TYR:CE2  | 1:A:82:ILE:HD12 | 0.41     | 2.50        | 4      | 3     |
| 1:A:68:ILE:CD1  | 1:A:79:TYR:CE2  | 0.41     | 3.03        | 35     | 4     |
| 1:A:74:ASP:OD1  | 1:A:74:ASP:O    | 0.41     | 2.38        | 35     | 1     |
| 1:A:36:ASP:N    | 1:A:36:ASP:OD2  | 0.41     | 2.50        | 40     | 1     |
| 1:A:18:ASN:N    | 1:A:18:ASN:ND2  | 0.41     | 2.67        | 1      | 1     |
| 1:A:58:ARG:NE   | 1:A:60:ASP:OD1  | 0.41     | 2.51        | 9      | 1     |
| 1:A:52:SER:C    | 1:A:54:LYS:H    | 0.40     | 2.22        | 19     | 1     |
| 1:A:49:LEU:HD22 | 1:A:55:TYR:CE1  | 0.40     | 2.51        | 32     | 1     |
| 1:A:24:HIS:ND1  | 1:A:24:HIS:O    | 0.40     | 2.55        | 40     | 1     |

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

| Mol | Chain | Analysed        | Favoured     | Allowed    | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|------------|------------|-------------|----|
| 1   | A     | 83/105 (79%)    | 77±1 (92±1%) | 5±1 (6±1%) | 1±0 (1±0%) | 11          | 58 |
| All | All   | 3320/4200 (79%) | 3061 (92%)   | 212 (6%)   | 47 (1%)    | 11          | 58 |

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 16  | ILE  | 40             |
| 1   | A     | 15  | ARG  | 5              |
| 1   | A     | 25  | GLN  | 2              |

### 6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

| Mol | Chain | Analysed        | Rotameric    | Outliers   | Percentiles |
|-----|-------|-----------------|--------------|------------|-------------|
| 1   | A     | 74/92 (80%)     | 72±1 (97±1%) | 2±1 (3±1%) | 41 88       |
| All | All   | 2960/3680 (80%) | 2882 (97%)   | 78 (3%)    | 41 88       |

All 4 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 31  | CYS  | 40             |
| 1   | A     | 48  | GLU  | 25             |
| 1   | A     | 72  | THR  | 12             |
| 1   | A     | 64  | HIS  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 6.7 Other polymers ⓘ

There are no such molecules in this entry.

## 6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 90% for the entire structure.

### 7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch\_output*

#### 7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

|                                         |      |
|-----------------------------------------|------|
| Total number of shifts                  | 1270 |
| Number of shifts mapped to atoms        | 1270 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 1    |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 103      | $0.12 \pm 0.11$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 97       | $-0.10 \pm 0.13$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 96       | $0.03 \pm 0.15$                 | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 97       | $0.12 \pm 0.41$                 | None needed ( $< 0.5$ ppm) |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 92%, i.e. 1018 atoms were assigned a chemical shift out of a possible 1109. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 407/415 (98%) | 167/168 (99%) | 160/166 (96%)   | 80/81 (99%)     |
| Sidechain | 525/585 (90%) | 354/376 (94%) | 164/185 (89%)   | 7/24 (29%)      |

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|          | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|----------|-----------------|----------------------|-----------------------|-----------------------|
| Aromatic | 86/109 (79%)    | 45/54 (83%)          | 40/51 (78%)           | 1/4 (25%)             |
| Overall  | 1018/1109 (92%) | 566/598 (95%)        | 364/402 (91%)         | 88/109 (81%)          |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 1269 atoms were assigned a chemical shift out of a possible 1403. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|-----------|-----------------|----------------------|-----------------------|-----------------------|
| Backbone  | 505/522 (97%)   | 209/212 (99%)        | 199/210 (95%)         | 97/100 (97%)          |
| Sidechain | 670/762 (88%)   | 452/490 (92%)        | 209/239 (87%)         | 9/33 (27%)            |
| Aromatic  | 94/119 (79%)    | 49/59 (83%)          | 44/56 (79%)           | 1/4 (25%)             |
| Overall   | 1269/1403 (90%) | 710/761 (93%)        | 452/505 (90%)         | 107/137 (78%)         |

#### 7.1.4 Statistically unusual chemical shifts [i](#)

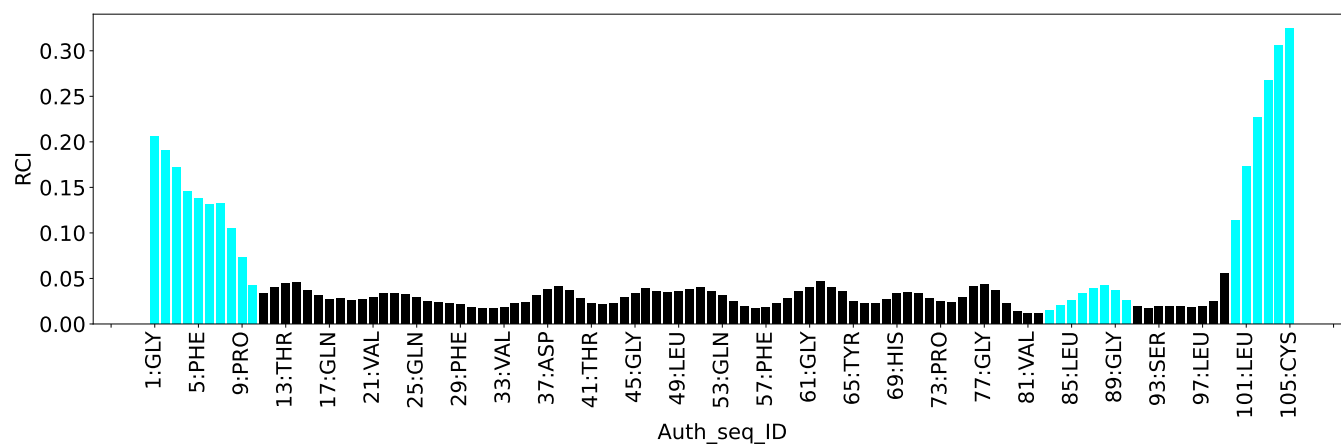
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 66  | MET  | HB3  | -0.28      | 0.33 – 3.66         | -6.8    |

#### 7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:





## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 6441  |
| Intra-residue ( $ i-j =0$ )                              | 3178  |
| Sequential ( $ i-j =1$ )                                 | 1234  |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 314   |
| Long range ( $ i-j \geq 5$ )                             | 1715  |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 189   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 63.1  |
| Number of long range restraints per residue <sup>1</sup> | 16.3  |

<sup>1</sup>Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

### 8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

#### 8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|----------------------------------------|---------|
| 0.1-0.2 (Small)  | 408.0                                  | 0.2     |
| 0.2-0.5 (Medium) | 164.3                                  | 0.5     |
| >0.5 (Large)     | 7.2                                    | 3.29    |

### 8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation.

| Bins (°)           | Average number of violations per model | Max (°) |
|--------------------|----------------------------------------|---------|
| 1.0-10.0 (Small)   | 23.4                                   | 6.1     |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

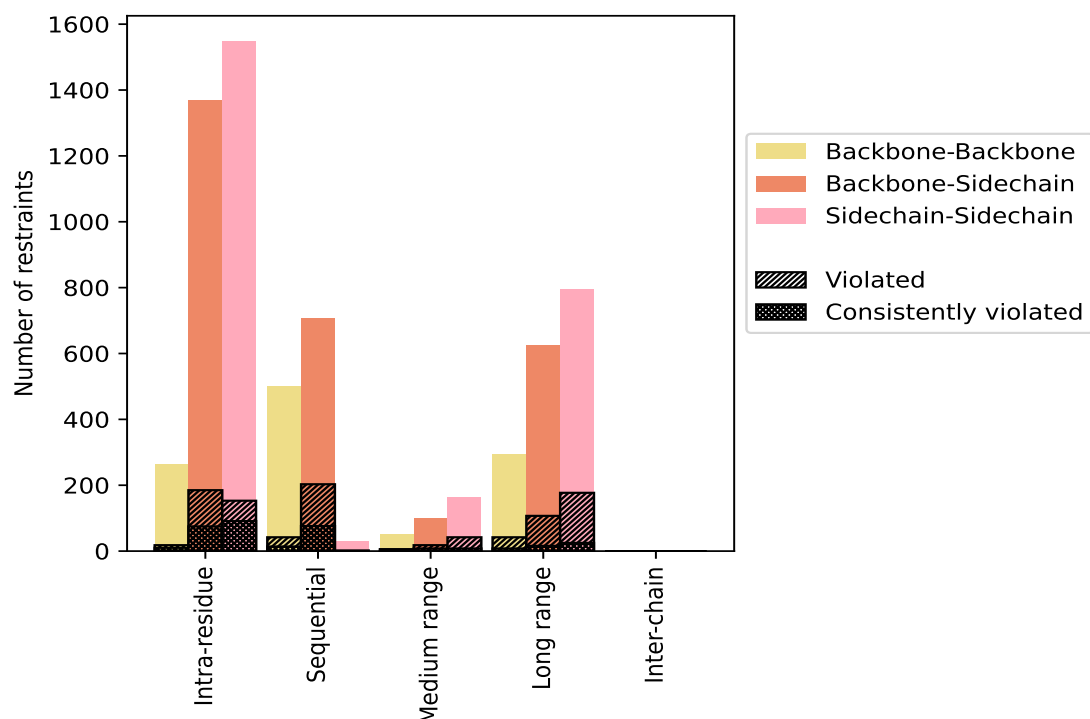
### 9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

| Restrains type                                             | Count                | % <sup>1</sup>        | Violated <sup>3</sup> |                      |                      | Consistently Violated <sup>4</sup> |                     |                     |
|------------------------------------------------------------|----------------------|-----------------------|-----------------------|----------------------|----------------------|------------------------------------|---------------------|---------------------|
|                                                            |                      |                       | Count                 | % <sup>2</sup>       | % <sup>1</sup>       | Count                              | % <sup>2</sup>      | % <sup>1</sup>      |
| <a href="#">Intra-residue ( i-j =0)</a>                    | <a href="#">3178</a> | <a href="#">49.3</a>  | <a href="#">356</a>   | <a href="#">11.2</a> | <a href="#">5.5</a>  | <a href="#">176</a>                | <a href="#">5.5</a> | <a href="#">2.7</a> |
| Backbone-Backbone                                          | 262                  | 4.1                   | 18                    | 6.9                  | 0.3                  | 10                                 | 3.8                 | 0.2                 |
| Backbone-Sidechain                                         | 1368                 | 21.2                  | 185                   | 13.5                 | 2.9                  | 75                                 | 5.5                 | 1.2                 |
| Sidechain-Sidechain                                        | 1548                 | 24.0                  | 153                   | 9.9                  | 2.4                  | 91                                 | 5.9                 | 1.4                 |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">1234</a> | <a href="#">19.2</a>  | <a href="#">247</a>   | <a href="#">20.0</a> | <a href="#">3.8</a>  | <a href="#">90</a>                 | <a href="#">7.3</a> | <a href="#">1.4</a> |
| Backbone-Backbone                                          | 499                  | 7.7                   | 42                    | 8.4                  | 0.7                  | 14                                 | 2.8                 | 0.2                 |
| Backbone-Sidechain                                         | 707                  | 11.0                  | 203                   | 28.7                 | 3.2                  | 76                                 | 10.7                | 1.2                 |
| Sidechain-Sidechain                                        | 28                   | 0.4                   | 2                     | 7.1                  | 0.0                  | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">314</a>  | <a href="#">4.9</a>   | <a href="#">66</a>    | <a href="#">21.0</a> | <a href="#">1.0</a>  | <a href="#">17</a>                 | <a href="#">5.4</a> | <a href="#">0.3</a> |
| Backbone-Backbone                                          | 50                   | 0.8                   | 6                     | 12.0                 | 0.1                  | 1                                  | 2.0                 | 0.0                 |
| Backbone-Sidechain                                         | 100                  | 1.6                   | 18                    | 18.0                 | 0.3                  | 8                                  | 8.0                 | 0.1                 |
| Sidechain-Sidechain                                        | 164                  | 2.5                   | 42                    | 25.6                 | 0.7                  | 8                                  | 4.9                 | 0.1                 |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">1715</a> | <a href="#">26.6</a>  | <a href="#">326</a>   | <a href="#">19.0</a> | <a href="#">5.1</a>  | <a href="#">49</a>                 | <a href="#">2.9</a> | <a href="#">0.8</a> |
| Backbone-Backbone                                          | 295                  | 4.6                   | 42                    | 14.2                 | 0.7                  | 8                                  | 2.7                 | 0.1                 |
| Backbone-Sidechain                                         | 626                  | 9.7                   | 107                   | 17.1                 | 1.7                  | 16                                 | 2.6                 | 0.2                 |
| Sidechain-Sidechain                                        | 794                  | 12.3                  | 177                   | 22.3                 | 2.7                  | 25                                 | 3.1                 | 0.4                 |
| <a href="#">Inter-chain</a>                                | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 0                    | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 0                    | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 0                    | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Hydrogen bond</a>                              | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| <a href="#">Disulfide bond</a>                             | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| <a href="#">Total</a>                                      | <a href="#">6441</a> | <a href="#">100.0</a> | <a href="#">995</a>   | <a href="#">15.4</a> | <a href="#">15.4</a> | <a href="#">332</a>                | <a href="#">5.2</a> | <a href="#">5.2</a> |
| Backbone-Backbone                                          | 1106                 | 17.2                  | 108                   | 9.8                  | 1.7                  | 33                                 | 3.0                 | 0.5                 |
| Backbone-Sidechain                                         | 2801                 | 43.5                  | 513                   | 18.3                 | 8.0                  | 175                                | 6.2                 | 2.7                 |
| Sidechain-Sidechain                                        | 2534                 | 39.3                  | 374                   | 14.8                 | 5.8                  | 124                                | 4.9                 | 1.9                 |

<sup>1</sup> percentage calculated with respect to the total number of distance restraints, <sup>2</sup> percentage calculated with respect to the number of restraints in a particular restraint category, <sup>3</sup> violated in at least one model, <sup>4</sup> violated in all the models

### 9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

## 9.2 Distance violation statistics for each model [i](#)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 239                  | 163             | 38              | 163             | 0               | 603   | 0.21     | 3.23    | 0.23                | 0.17       |
| 2        | 245                  | 158             | 37              | 146             | 0               | 586   | 0.21     | 3.2     | 0.25                | 0.17       |
| 3        | 237                  | 168             | 41              | 164             | 0               | 610   | 0.19     | 3.27    | 0.19                | 0.17       |
| 4        | 245                  | 168             | 38              | 165             | 0               | 616   | 0.2      | 3.22    | 0.22                | 0.16       |
| 5        | 247                  | 160             | 36              | 171             | 0               | 614   | 0.2      | 3.23    | 0.22                | 0.17       |
| 6        | 255                  | 166             | 35              | 156             | 0               | 612   | 0.2      | 3.24    | 0.23                | 0.17       |
| 7        | 247                  | 159             | 39              | 154             | 0               | 599   | 0.2      | 3.24    | 0.23                | 0.17       |
| 8        | 245                  | 172             | 38              | 154             | 0               | 609   | 0.2      | 3.22    | 0.22                | 0.17       |
| 9        | 241                  | 152             | 37              | 154             | 0               | 584   | 0.2      | 3.26    | 0.25                | 0.17       |
| 10       | 249                  | 162             | 43              | 158             | 0               | 612   | 0.2      | 3.24    | 0.23                | 0.16       |

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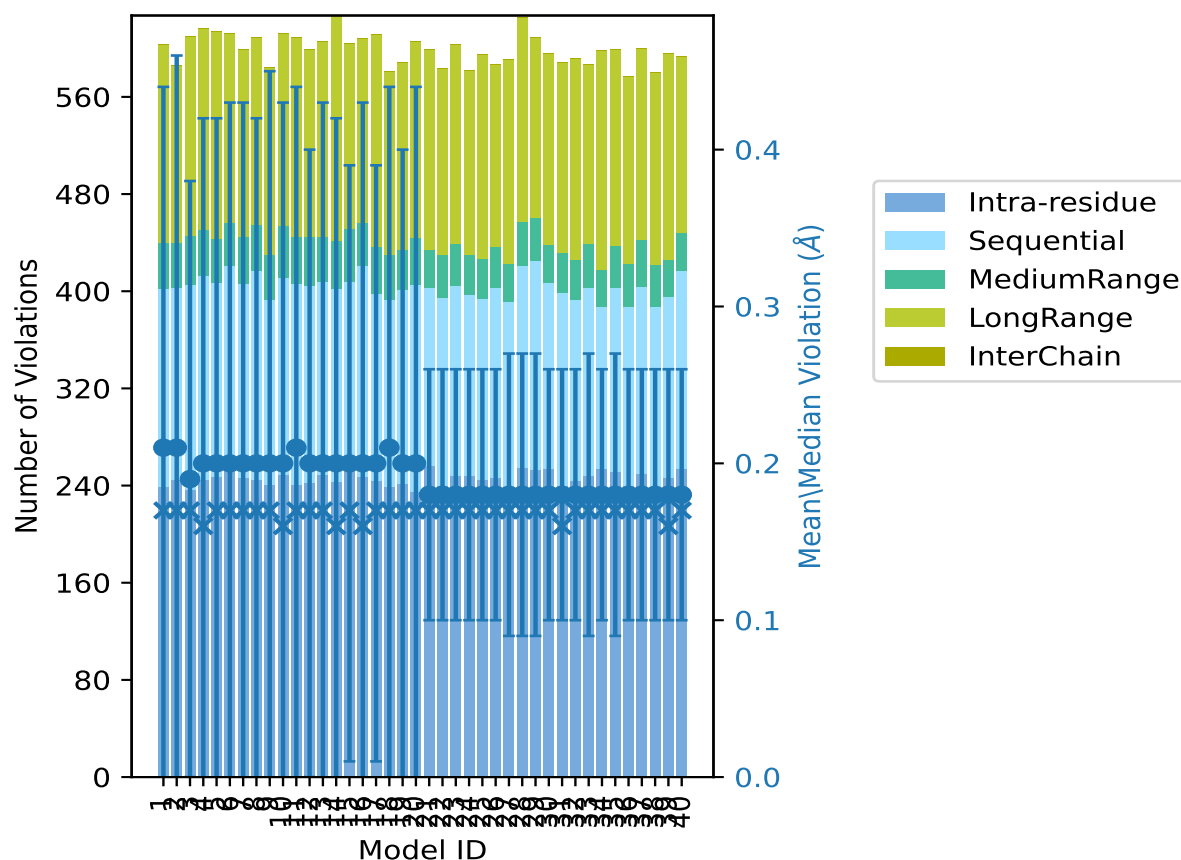
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 241                  | 165             | 39              | 164             | 0               | 609   | 0.21     | 3.26    | 0.23                | 0.17       |
| 12       | 242                  | 162             | 41              | 154             | 0               | 599   | 0.2      | 3.26    | 0.2                 | 0.17       |
| 13       | 249                  | 159             | 37              | 161             | 0               | 606   | 0.2      | 3.26    | 0.23                | 0.17       |
| 14       | 243                  | 159             | 39              | 186             | 0               | 627   | 0.2      | 3.24    | 0.22                | 0.16       |
| 15       | 255                  | 153             | 43              | 153             | 0               | 604   | 0.2      | 3.24    | 0.19                | 0.17       |
| 16       | 247                  | 174             | 35              | 152             | 0               | 608   | 0.2      | 3.29    | 0.23                | 0.16       |
| 17       | 244                  | 154             | 39              | 174             | 0               | 611   | 0.2      | 3.24    | 0.19                | 0.17       |
| 18       | 239                  | 154             | 37              | 151             | 0               | 581   | 0.21     | 3.27    | 0.23                | 0.17       |
| 19       | 242                  | 159             | 33              | 154             | 0               | 588   | 0.2      | 3.27    | 0.2                 | 0.17       |
| 20       | 235                  | 170             | 39              | 162             | 0               | 606   | 0.2      | 3.23    | 0.24                | 0.17       |
| 21       | 256                  | 147             | 31              | 165             | 0               | 599   | 0.18     | 1.46    | 0.08                | 0.17       |
| 22       | 240                  | 155             | 35              | 153             | 0               | 583   | 0.18     | 1.53    | 0.08                | 0.17       |
| 23       | 248                  | 157             | 34              | 164             | 0               | 603   | 0.18     | 1.56    | 0.08                | 0.17       |
| 24       | 248                  | 149             | 33              | 152             | 0               | 582   | 0.18     | 1.46    | 0.08                | 0.17       |
| 25       | 245                  | 149             | 33              | 168             | 0               | 595   | 0.18     | 1.49    | 0.08                | 0.17       |
| 26       | 246                  | 157             | 34              | 150             | 0               | 587   | 0.18     | 1.53    | 0.08                | 0.17       |
| 27       | 238                  | 153             | 32              | 168             | 0               | 591   | 0.18     | 1.51    | 0.09                | 0.17       |
| 28       | 255                  | 166             | 36              | 168             | 0               | 625   | 0.18     | 1.52    | 0.09                | 0.17       |
| 29       | 253                  | 172             | 35              | 149             | 0               | 609   | 0.18     | 1.61    | 0.09                | 0.17       |
| 30       | 254                  | 153             | 31              | 158             | 0               | 596   | 0.18     | 1.5     | 0.08                | 0.17       |
| 31       | 240                  | 159             | 33              | 156             | 0               | 588   | 0.18     | 1.53    | 0.08                | 0.16       |
| 32       | 244                  | 149             | 33              | 166             | 0               | 592   | 0.18     | 1.47    | 0.08                | 0.17       |
| 33       | 248                  | 155             | 36              | 148             | 0               | 587   | 0.18     | 1.57    | 0.09                | 0.17       |
| 34       | 254                  | 133             | 31              | 180             | 0               | 598   | 0.18     | 1.49    | 0.08                | 0.17       |
| 35       | 251                  | 152             | 34              | 162             | 0               | 599   | 0.18     | 1.54    | 0.09                | 0.17       |
| 36       | 240                  | 147             | 36              | 154             | 0               | 577   | 0.18     | 1.53    | 0.08                | 0.17       |
| 37       | 250                  | 154             | 38              | 158             | 0               | 600   | 0.18     | 1.55    | 0.08                | 0.17       |
| 38       | 238                  | 149             | 35              | 158             | 0               | 580   | 0.18     | 1.48    | 0.08                | 0.17       |
| 39       | 246                  | 149             | 31              | 170             | 0               | 596   | 0.18     | 1.49    | 0.08                | 0.16       |
| 40       | 254                  | 163             | 31              | 145             | 0               | 593   | 0.18     | 1.51    | 0.08                | 0.17       |

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

### 9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

### 9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 5446(IR:2822, SQ:987, MR:248, LR:1389, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |      |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %    |
| 26                            | 23              | 4               | 42              | 0               | 95    | 1                        | 2.5  |
| 18                            | 8               | 4               | 21              | 0               | 51    | 2                        | 5.0  |
| 10                            | 6               | 2               | 8               | 0               | 26    | 3                        | 7.5  |
| 6                             | 14              | 3               | 8               | 0               | 31    | 4                        | 10.0 |
| 8                             | 4               | 2               | 18              | 0               | 32    | 5                        | 12.5 |
| 10                            | 4               | 2               | 11              | 0               | 27    | 6                        | 15.0 |

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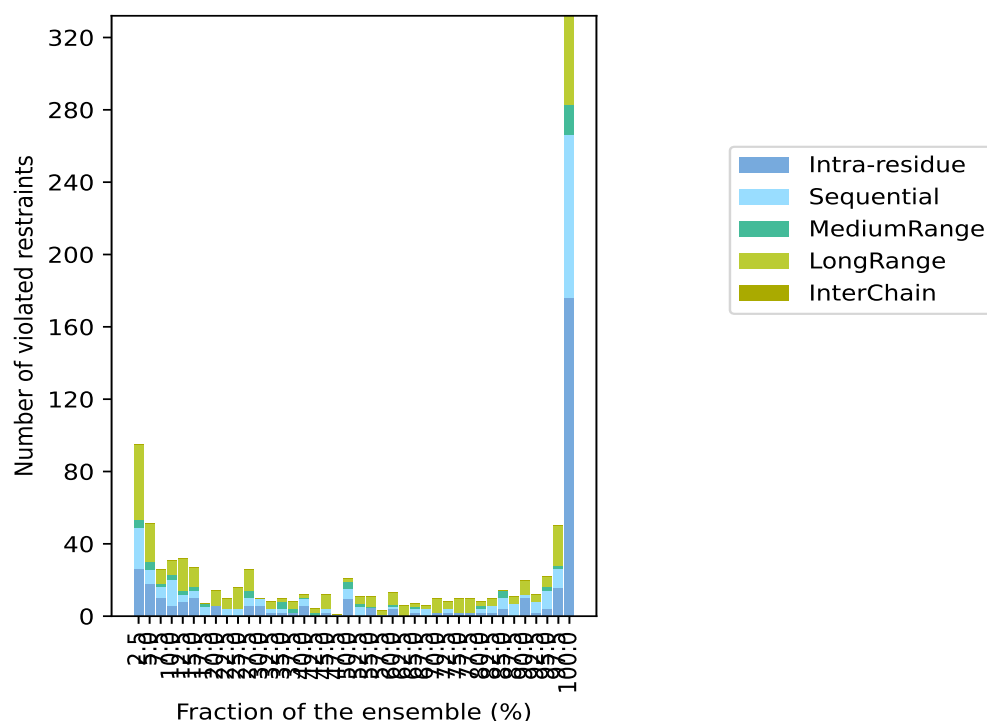
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 1                             | 4               | 2               | 0               | 0               | 7     | 7                        | 17.5  |
| 6                             | 0               | 0               | 8               | 0               | 14    | 8                        | 20.0  |
| 0                             | 4               | 0               | 6               | 0               | 10    | 9                        | 22.5  |
| 0                             | 4               | 0               | 12              | 0               | 16    | 10                       | 25.0  |
| 6                             | 4               | 4               | 12              | 0               | 26    | 11                       | 27.5  |
| 6                             | 4               | 0               | 0               | 0               | 10    | 12                       | 30.0  |
| 2                             | 2               | 0               | 4               | 0               | 8     | 13                       | 32.5  |
| 2                             | 2               | 4               | 2               | 0               | 10    | 14                       | 35.0  |
| 2                             | 0               | 2               | 4               | 0               | 8     | 15                       | 37.5  |
| 6                             | 4               | 0               | 2               | 0               | 12    | 16                       | 40.0  |
| 0                             | 0               | 2               | 2               | 0               | 4     | 17                       | 42.5  |
| 2                             | 2               | 0               | 8               | 0               | 12    | 18                       | 45.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 19                       | 47.5  |
| 10                            | 5               | 4               | 2               | 0               | 21    | 20                       | 50.0  |
| 0                             | 5               | 2               | 4               | 0               | 11    | 21                       | 52.5  |
| 5                             | 0               | 0               | 6               | 0               | 11    | 22                       | 55.0  |
| 0                             | 1               | 0               | 2               | 0               | 3     | 23                       | 57.5  |
| 4                             | 1               | 1               | 7               | 0               | 13    | 24                       | 60.0  |
| 0                             | 0               | 0               | 6               | 0               | 6     | 25                       | 62.5  |
| 2                             | 2               | 1               | 2               | 0               | 7     | 26                       | 65.0  |
| 0                             | 4               | 0               | 2               | 0               | 6     | 27                       | 67.5  |
| 2                             | 0               | 0               | 8               | 0               | 10    | 28                       | 70.0  |
| 2                             | 2               | 0               | 4               | 0               | 8     | 29                       | 72.5  |
| 2                             | 0               | 0               | 8               | 0               | 10    | 30                       | 75.0  |
| 2                             | 0               | 0               | 8               | 0               | 10    | 31                       | 77.5  |
| 2                             | 2               | 2               | 2               | 0               | 8     | 32                       | 80.0  |
| 2                             | 4               | 0               | 4               | 0               | 10    | 33                       | 82.5  |
| 4                             | 6               | 4               | 0               | 0               | 14    | 34                       | 85.0  |
| 0                             | 7               | 0               | 4               | 0               | 11    | 35                       | 87.5  |
| 10                            | 2               | 0               | 8               | 0               | 20    | 36                       | 90.0  |
| 2                             | 6               | 0               | 4               | 0               | 12    | 37                       | 92.5  |
| 4                             | 10              | 2               | 6               | 0               | 22    | 38                       | 95.0  |
| 16                            | 10              | 2               | 22              | 0               | 50    | 39                       | 97.5  |
| 176                           | 90              | 17              | 49              | 0               | 332   | 40                       | 100.0 |

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)

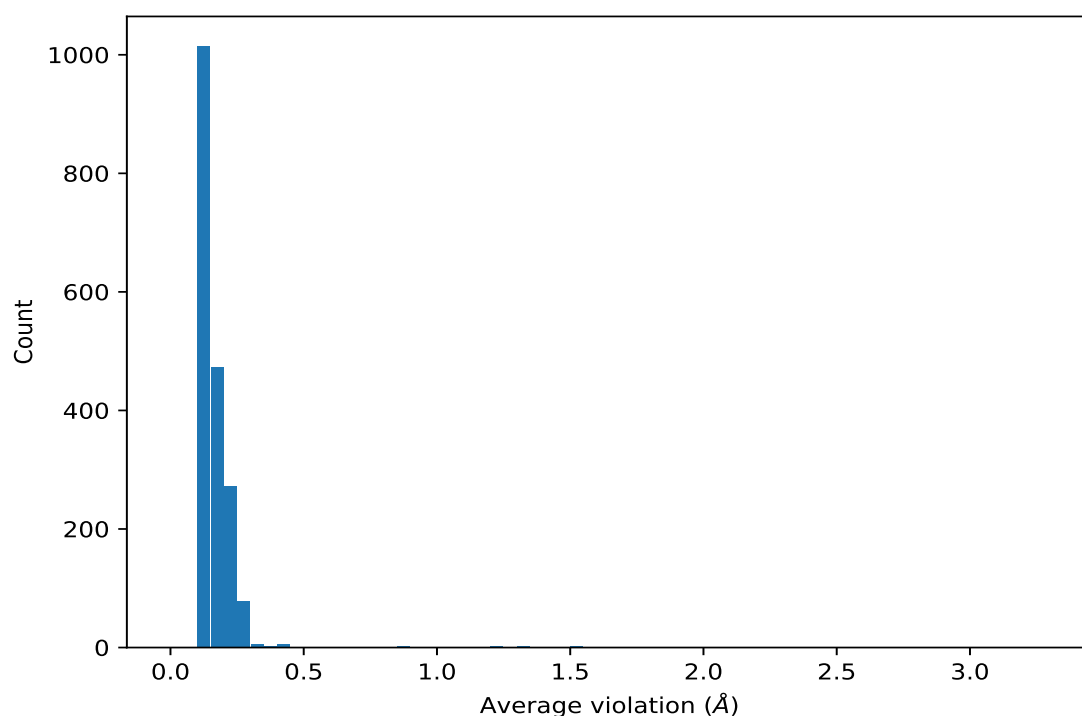


## 9.4 Most violated distance restraints in the ensemble [i](#)

### 9.4.1 Histogram : Distribution of mean distance violations [i](#)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble





#### 9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

| Key      | Atom-1          | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 40                  | 1.52     | 0.03                | 1.52       |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 40                  | 1.52     | 0.03                | 1.52       |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 40                  | 1.52     | 0.03                | 1.52       |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 40                  | 0.87     | 0.1                 | 0.88       |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 40                  | 0.87     | 0.1                 | 0.88       |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 40                  | 0.87     | 0.1                 | 0.88       |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 40                  | 0.51     | 0.04                | 0.52       |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 40                  | 0.41     | 0.02                | 0.41       |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 40                  | 0.41     | 0.02                | 0.41       |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 40                  | 0.41     | 0.02                | 0.41       |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2 | 40                  | 0.39     | 0.05                | 0.39       |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 40                  | 0.39     | 0.06                | 0.4        |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 40                  | 0.32     | 0.03                | 0.32       |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 40                  | 0.32     | 0.03                | 0.32       |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 40                  | 0.32     | 0.03                | 0.32       |
| (1,123)  | 1:55:A:TYR:H    | 1:54:A:LYS:H   | 40                  | 0.3      | 0.02                | 0.3        |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (3,125)  | 1:55:A:TYR:H    | 1:54:A:LYS:H    | 40                  | 0.3      | 0.02                | 0.3        |
| (3,2485) | 1:9:A:PRO:HD3   | 1:9:A:PRO:HB3   | 40                  | 0.29     | 0.06                | 0.31       |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 40                  | 0.29     | 0.0                 | 0.29       |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 40                  | 0.29     | 0.0                 | 0.29       |
| (1,3170) | 1:5:A:PHE:HD1   | 1:5:A:PHE:HE1   | 40                  | 0.29     | 0.0                 | 0.29       |
| (1,3170) | 1:5:A:PHE:HD1   | 1:5:A:PHE:HE2   | 40                  | 0.29     | 0.0                 | 0.29       |
| (1,3170) | 1:5:A:PHE:HD2   | 1:5:A:PHE:HE1   | 40                  | 0.29     | 0.0                 | 0.29       |
| (1,3170) | 1:5:A:PHE:HD2   | 1:5:A:PHE:HE2   | 40                  | 0.29     | 0.0                 | 0.29       |
| (3,3176) | 1:5:A:PHE:HD1   | 1:5:A:PHE:HE1   | 40                  | 0.29     | 0.0                 | 0.29       |
| (3,3176) | 1:5:A:PHE:HD1   | 1:5:A:PHE:HE2   | 40                  | 0.29     | 0.0                 | 0.29       |
| (3,3176) | 1:5:A:PHE:HD2   | 1:5:A:PHE:HE1   | 40                  | 0.29     | 0.0                 | 0.29       |
| (3,3176) | 1:5:A:PHE:HD2   | 1:5:A:PHE:HE2   | 40                  | 0.29     | 0.0                 | 0.29       |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 40                  | 0.28     | 0.01                | 0.28       |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 40                  | 0.28     | 0.01                | 0.28       |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD23 | 40                  | 0.28     | 0.01                | 0.28       |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 40                  | 0.28     | 0.01                | 0.28       |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 40                  | 0.28     | 0.01                | 0.28       |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 40                  | 0.28     | 0.01                | 0.28       |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 40                  | 0.28     | 0.01                | 0.28       |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 40                  | 0.28     | 0.01                | 0.28       |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD23 | 40                  | 0.28     | 0.01                | 0.28       |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 40                  | 0.28     | 0.01                | 0.28       |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 40                  | 0.28     | 0.01                | 0.28       |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 40                  | 0.28     | 0.01                | 0.28       |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 40                  | 0.28     | 0.0                 | 0.28       |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 40                  | 0.28     | 0.0                 | 0.28       |
| (1,584)  | 1:93:A:SER:H    | 1:92:A:ARG:HB2  | 40                  | 0.28     | 0.02                | 0.28       |
| (3,584)  | 1:93:A:SER:H    | 1:92:A:ARG:HB2  | 40                  | 0.28     | 0.02                | 0.28       |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3  | 40                  | 0.27     | 0.1                 | 0.29       |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3  | 40                  | 0.27     | 0.1                 | 0.29       |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3  | 40                  | 0.27     | 0.1                 | 0.29       |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 40                  | 0.26     | 0.0                 | 0.26       |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 40                  | 0.26     | 0.0                 | 0.26       |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 40                  | 0.26     | 0.0                 | 0.26       |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 40                  | 0.26     | 0.0                 | 0.26       |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 40                  | 0.26     | 0.0                 | 0.26       |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 40                  | 0.26     | 0.0                 | 0.26       |
| (1,176)  | 1:10:A:ILE:H    | 1:35:A:PHE:HD1  | 40                  | 0.26     | 0.04                | 0.25       |
| (1,176)  | 1:10:A:ILE:H    | 1:35:A:PHE:HD2  | 40                  | 0.26     | 0.04                | 0.25       |
| (3,176)  | 1:10:A:ILE:H    | 1:35:A:PHE:HD1  | 40                  | 0.26     | 0.04                | 0.25       |
| (3,176)  | 1:10:A:ILE:H    | 1:35:A:PHE:HD2  | 40                  | 0.26     | 0.04                | 0.25       |
| (1,2285) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H    | 40                  | 0.26     | 0.01                | 0.26       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (3,2288) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H    | 40                  | 0.26     | 0.01                | 0.26       |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 40                  | 0.26     | 0.01                | 0.26       |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 40                  | 0.26     | 0.01                | 0.26       |
| (1,2213) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1  | 40                  | 0.25     | 0.01                | 0.25       |
| (1,3159) | 1:42:A:TRP:HD1  | 1:42:A:TRP:HB3  | 40                  | 0.25     | 0.01                | 0.25       |
| (3,2216) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1  | 40                  | 0.25     | 0.01                | 0.25       |
| (3,3165) | 1:42:A:TRP:HD1  | 1:42:A:TRP:HB3  | 40                  | 0.25     | 0.01                | 0.25       |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 40                  | 0.25     | 0.02                | 0.26       |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 40                  | 0.25     | 0.02                | 0.26       |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 40                  | 0.25     | 0.02                | 0.26       |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 40                  | 0.25     | 0.02                | 0.26       |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 40                  | 0.25     | 0.02                | 0.26       |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 40                  | 0.25     | 0.02                | 0.26       |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 40                  | 0.25     | 0.02                | 0.26       |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 40                  | 0.25     | 0.02                | 0.26       |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 40                  | 0.25     | 0.02                | 0.26       |
| (1,2742) | 1:86:A:GLU:HG2  | 1:86:A:GLU:HG3  | 40                  | 0.25     | 0.0                 | 0.25       |
| (3,2746) | 1:86:A:GLU:HG2  | 1:86:A:GLU:HG3  | 40                  | 0.25     | 0.0                 | 0.25       |
| (1,1184) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 40                  | 0.25     | 0.02                | 0.24       |
| (3,1188) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 40                  | 0.25     | 0.02                | 0.24       |
| (1,2511) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2  | 40                  | 0.24     | 0.06                | 0.25       |
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2  | 40                  | 0.24     | 0.06                | 0.25       |
| (1,169)  | 1:10:A:ILE:H    | 1:10:A:ILE:HG12 | 40                  | 0.24     | 0.01                | 0.24       |
| (3,169)  | 1:10:A:ILE:H    | 1:10:A:ILE:HG12 | 40                  | 0.24     | 0.01                | 0.24       |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA   | 40                  | 0.24     | 0.02                | 0.24       |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA   | 40                  | 0.24     | 0.02                | 0.24       |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA   | 40                  | 0.24     | 0.02                | 0.24       |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA   | 40                  | 0.24     | 0.02                | 0.24       |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA   | 40                  | 0.24     | 0.02                | 0.24       |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA   | 40                  | 0.24     | 0.02                | 0.24       |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 40                  | 0.24     | 0.02                | 0.24       |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 40                  | 0.24     | 0.02                | 0.24       |
| (1,2667) | 1:25:A:GLN:HG2  | 1:25:A:GLN:HG3  | 40                  | 0.24     | 0.0                 | 0.24       |
| (3,2671) | 1:25:A:GLN:HG2  | 1:25:A:GLN:HG3  | 40                  | 0.24     | 0.0                 | 0.24       |
| (1,3046) | 1:57:A:PHE:HB3  | 1:57:A:PHE:H    | 40                  | 0.24     | 0.01                | 0.24       |
| (3,3054) | 1:57:A:PHE:HB3  | 1:57:A:PHE:H    | 40                  | 0.24     | 0.01                | 0.24       |
| (1,768)  | 1:75:A:ASP:H    | 1:75:A:ASP:HB3  | 40                  | 0.24     | 0.01                | 0.24       |
| (3,768)  | 1:75:A:ASP:H    | 1:75:A:ASP:HB3  | 40                  | 0.24     | 0.01                | 0.24       |
| (1,416)  | 1:96:A:GLU:H    | 1:96:A:GLU:HB3  | 40                  | 0.24     | 0.01                | 0.24       |
| (3,416)  | 1:96:A:GLU:H    | 1:96:A:GLU:HB3  | 40                  | 0.24     | 0.01                | 0.24       |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2  | 40                  | 0.24     | 0.01                | 0.24       |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2  | 40                  | 0.24     | 0.01                | 0.24       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2  | 40                  | 0.24     | 0.01                | 0.24       |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2  | 40                  | 0.24     | 0.01                | 0.24       |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA   | 40                  | 0.24     | 0.01                | 0.24       |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA   | 40                  | 0.24     | 0.01                | 0.24       |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA   | 40                  | 0.24     | 0.01                | 0.24       |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA   | 40                  | 0.24     | 0.01                | 0.24       |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA   | 40                  | 0.24     | 0.01                | 0.24       |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA   | 40                  | 0.24     | 0.01                | 0.24       |
| (1,2693) | 1:23:A:GLU:HA   | 1:24:A:HIS:H    | 40                  | 0.23     | 0.01                | 0.23       |
| (3,2697) | 1:23:A:GLU:HA   | 1:24:A:HIS:H    | 40                  | 0.23     | 0.01                | 0.23       |
| (1,3127) | 1:55:A:TYR:HD1  | 1:49:A:LEU:HB2  | 40                  | 0.23     | 0.03                | 0.23       |
| (1,3127) | 1:55:A:TYR:HD2  | 1:49:A:LEU:HB2  | 40                  | 0.23     | 0.03                | 0.23       |
| (3,3133) | 1:55:A:TYR:HD1  | 1:49:A:LEU:HB2  | 40                  | 0.23     | 0.03                | 0.23       |
| (3,3133) | 1:55:A:TYR:HD2  | 1:49:A:LEU:HB2  | 40                  | 0.23     | 0.03                | 0.23       |
| (1,2151) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3   | 40                  | 0.23     | 0.0                 | 0.23       |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3   | 40                  | 0.23     | 0.0                 | 0.23       |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 40                  | 0.23     | 0.02                | 0.24       |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 40                  | 0.23     | 0.02                | 0.24       |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 40                  | 0.23     | 0.02                | 0.24       |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 40                  | 0.23     | 0.02                | 0.24       |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 40                  | 0.23     | 0.02                | 0.24       |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 40                  | 0.23     | 0.02                | 0.24       |
| (1,2718) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 40                  | 0.23     | 0.01                | 0.23       |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 40                  | 0.23     | 0.01                | 0.23       |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 40                  | 0.23     | 0.0                 | 0.23       |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 40                  | 0.23     | 0.0                 | 0.23       |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 40                  | 0.23     | 0.0                 | 0.23       |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 40                  | 0.23     | 0.0                 | 0.23       |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2  | 40                  | 0.23     | 0.01                | 0.23       |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2  | 40                  | 0.23     | 0.01                | 0.23       |
| (1,129)  | 1:39:A:ILE:H    | 1:39:A:ILE:HA   | 40                  | 0.22     | 0.02                | 0.23       |
| (3,131)  | 1:39:A:ILE:H    | 1:39:A:ILE:HA   | 40                  | 0.22     | 0.02                | 0.23       |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB   | 40                  | 0.22     | 0.0                 | 0.22       |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB   | 40                  | 0.22     | 0.0                 | 0.22       |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB   | 40                  | 0.22     | 0.0                 | 0.22       |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB   | 40                  | 0.22     | 0.0                 | 0.22       |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB   | 40                  | 0.22     | 0.0                 | 0.22       |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB   | 40                  | 0.22     | 0.0                 | 0.22       |
| (1,969)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 40                  | 0.22     | 0.01                | 0.22       |
| (3,970)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 40                  | 0.22     | 0.01                | 0.22       |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3  | 40                  | 0.22     | 0.02                | 0.22       |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3  | 40                  | 0.22     | 0.02                | 0.22       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3  | 40                  | 0.22     | 0.02                | 0.22       |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3  | 40                  | 0.22     | 0.02                | 0.22       |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3  | 40                  | 0.22     | 0.02                | 0.22       |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3  | 40                  | 0.22     | 0.02                | 0.22       |
| (1,2668) | 1:25:A:GLN:HG3  | 1:25:A:GLN:HA   | 40                  | 0.22     | 0.01                | 0.22       |
| (3,2672) | 1:25:A:GLN:HG3  | 1:25:A:GLN:HA   | 40                  | 0.22     | 0.01                | 0.22       |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 40                  | 0.22     | 0.0                 | 0.22       |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 40                  | 0.22     | 0.0                 | 0.22       |
| (1,715)  | 1:16:A:ILE:H    | 1:15:A:ARG:HB3  | 40                  | 0.22     | 0.02                | 0.23       |
| (3,715)  | 1:16:A:ILE:H    | 1:15:A:ARG:HB3  | 40                  | 0.22     | 0.02                | 0.23       |
| (1,72)   | 1:51:A:GLU:H    | 1:50:A:THR:HG21 | 40                  | 0.22     | 0.01                | 0.22       |
| (1,72)   | 1:51:A:GLU:H    | 1:50:A:THR:HG22 | 40                  | 0.22     | 0.01                | 0.22       |
| (1,72)   | 1:51:A:GLU:H    | 1:50:A:THR:HG23 | 40                  | 0.22     | 0.01                | 0.22       |
| (3,74)   | 1:51:A:GLU:H    | 1:50:A:THR:HG21 | 40                  | 0.22     | 0.01                | 0.22       |
| (3,74)   | 1:51:A:GLU:H    | 1:50:A:THR:HG22 | 40                  | 0.22     | 0.01                | 0.22       |
| (3,74)   | 1:51:A:GLU:H    | 1:50:A:THR:HG23 | 40                  | 0.22     | 0.01                | 0.22       |
| (1,2796) | 1:15:A:ARG:HG3  | 1:15:A:ARG:HB3  | 40                  | 0.21     | 0.0                 | 0.21       |
| (1,2857) | 1:92:A:ARG:HB3  | 1:92:A:ARG:HG3  | 40                  | 0.21     | 0.0                 | 0.21       |
| (3,2803) | 1:15:A:ARG:HG3  | 1:15:A:ARG:HB3  | 40                  | 0.21     | 0.0                 | 0.21       |
| (3,2864) | 1:92:A:ARG:HB3  | 1:92:A:ARG:HG3  | 40                  | 0.21     | 0.0                 | 0.21       |
| (1,1778) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H    | 40                  | 0.21     | 0.04                | 0.22       |
| (3,1781) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H    | 40                  | 0.21     | 0.04                | 0.22       |
| (1,343)  | 1:14:A:LYS:H    | 1:33:A:VAL:HA   | 40                  | 0.21     | 0.03                | 0.21       |
| (3,343)  | 1:14:A:LYS:H    | 1:33:A:VAL:HA   | 40                  | 0.21     | 0.03                | 0.21       |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H    | 40                  | 0.21     | 0.01                | 0.21       |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H    | 40                  | 0.21     | 0.01                | 0.21       |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H    | 40                  | 0.21     | 0.01                | 0.21       |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H    | 40                  | 0.21     | 0.01                | 0.21       |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H    | 40                  | 0.21     | 0.01                | 0.21       |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H    | 40                  | 0.21     | 0.01                | 0.21       |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H    | 40                  | 0.21     | 0.01                | 0.21       |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H    | 40                  | 0.21     | 0.01                | 0.21       |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H    | 40                  | 0.21     | 0.01                | 0.21       |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H    | 40                  | 0.21     | 0.01                | 0.21       |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H    | 40                  | 0.21     | 0.01                | 0.21       |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H    | 40                  | 0.21     | 0.01                | 0.21       |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H    | 40                  | 0.21     | 0.04                | 0.2        |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H    | 40                  | 0.21     | 0.04                | 0.2        |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H    | 40                  | 0.21     | 0.04                | 0.2        |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H    | 40                  | 0.21     | 0.04                | 0.2        |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H    | 40                  | 0.21     | 0.04                | 0.2        |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H    | 40                  | 0.21     | 0.04                | 0.2        |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,739)  | 1:15:A:ARG:H    | 1:14:A:LYS:HB2  | 40                  | 0.21     | 0.02                | 0.21       |
| (3,739)  | 1:15:A:ARG:H    | 1:14:A:LYS:HB2  | 40                  | 0.21     | 0.02                | 0.21       |
| (1,2626) | 1:11:A:GLN:HG2  | 1:11:A:GLN:HB2  | 40                  | 0.21     | 0.0                 | 0.21       |
| (3,2630) | 1:11:A:GLN:HG2  | 1:11:A:GLN:HB2  | 40                  | 0.21     | 0.0                 | 0.21       |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 40                  | 0.21     | 0.03                | 0.21       |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 40                  | 0.21     | 0.03                | 0.21       |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 40                  | 0.21     | 0.03                | 0.21       |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 40                  | 0.21     | 0.03                | 0.21       |
| (1,1812) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 40                  | 0.21     | 0.01                | 0.21       |
| (1,1825) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 40                  | 0.21     | 0.01                | 0.21       |
| (3,1815) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 40                  | 0.21     | 0.01                | 0.21       |
| (3,1828) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 40                  | 0.21     | 0.01                | 0.21       |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 40                  | 0.2      | 0.02                | 0.2        |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 40                  | 0.2      | 0.02                | 0.2        |
| (1,556)  | 1:47:A:THR:H    | 1:48:A:GLU:H    | 40                  | 0.2      | 0.01                | 0.2        |
| (3,556)  | 1:47:A:THR:H    | 1:48:A:GLU:H    | 40                  | 0.2      | 0.01                | 0.2        |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 40                  | 0.2      | 0.02                | 0.2        |
| (3,1173) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 40                  | 0.2      | 0.02                | 0.2        |
| (1,525)  | 1:99:A:GLY:H    | 1:100:A:GLU:H   | 40                  | 0.2      | 0.03                | 0.19       |
| (1,2734) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2  | 40                  | 0.2      | 0.0                 | 0.2        |
| (3,525)  | 1:99:A:GLY:H    | 1:100:A:GLU:H   | 40                  | 0.2      | 0.03                | 0.19       |
| (3,2738) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2  | 40                  | 0.2      | 0.0                 | 0.2        |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 40                  | 0.2      | 0.03                | 0.2        |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 40                  | 0.2      | 0.03                | 0.2        |
| (1,3047) | 1:57:A:PHE:HB3  | 1:42:A:TRP:HE1  | 40                  | 0.2      | 0.03                | 0.19       |
| (3,3055) | 1:57:A:PHE:HB3  | 1:42:A:TRP:HE1  | 40                  | 0.2      | 0.03                | 0.19       |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 40                  | 0.2      | 0.02                | 0.2        |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 40                  | 0.2      | 0.02                | 0.2        |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 40                  | 0.2      | 0.02                | 0.2        |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 40                  | 0.2      | 0.02                | 0.2        |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 40                  | 0.2      | 0.02                | 0.2        |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 40                  | 0.2      | 0.02                | 0.2        |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 40                  | 0.2      | 0.01                | 0.2        |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 40                  | 0.2      | 0.01                | 0.2        |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 40                  | 0.2      | 0.01                | 0.2        |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 40                  | 0.2      | 0.01                | 0.2        |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 40                  | 0.2      | 0.01                | 0.2        |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 40                  | 0.2      | 0.01                | 0.2        |
| (1,2286) | 1:96:A:GLU:HG2  | 1:97:A:LEU:H    | 40                  | 0.2      | 0.02                | 0.2        |
| (3,2289) | 1:96:A:GLU:HG2  | 1:97:A:LEU:H    | 40                  | 0.2      | 0.02                | 0.2        |
| (1,1740) | 1:51:A:GLU:HG2  | 1:51:A:GLU:HB2  | 40                  | 0.2      | 0.0                 | 0.2        |
| (3,1743) | 1:51:A:GLU:HG2  | 1:51:A:GLU:HB2  | 40                  | 0.2      | 0.0                 | 0.2        |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1396) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA   | 40                  | 0.2      | 0.02                | 0.2        |
| (1,1396) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA   | 40                  | 0.2      | 0.02                | 0.2        |
| (1,1396) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA   | 40                  | 0.2      | 0.02                | 0.2        |
| (3,1400) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA   | 40                  | 0.2      | 0.02                | 0.2        |
| (3,1400) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA   | 40                  | 0.2      | 0.02                | 0.2        |
| (3,1400) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA   | 40                  | 0.2      | 0.02                | 0.2        |
| (1,133)  | 1:39:A:ILE:H    | 1:39:A:ILE:HG13 | 40                  | 0.2      | 0.02                | 0.19       |
| (1,2867) | 1:92:A:ARG:HD2  | 1:92:A:ARG:HG2  | 40                  | 0.2      | 0.0                 | 0.2        |
| (3,135)  | 1:39:A:ILE:H    | 1:39:A:ILE:HG13 | 40                  | 0.2      | 0.02                | 0.19       |
| (3,2874) | 1:92:A:ARG:HD2  | 1:92:A:ARG:HG2  | 40                  | 0.2      | 0.0                 | 0.2        |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3  | 40                  | 0.2      | 0.02                | 0.2        |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3  | 40                  | 0.2      | 0.02                | 0.2        |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3  | 40                  | 0.2      | 0.02                | 0.2        |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3  | 40                  | 0.2      | 0.02                | 0.2        |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3  | 40                  | 0.2      | 0.02                | 0.2        |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3  | 40                  | 0.2      | 0.02                | 0.2        |
| (1,814)  | 1:25:A:GLN:H    | 1:71:A:VAL:HG21 | 40                  | 0.2      | 0.03                | 0.2        |
| (1,814)  | 1:25:A:GLN:H    | 1:71:A:VAL:HG22 | 40                  | 0.2      | 0.03                | 0.2        |
| (1,814)  | 1:25:A:GLN:H    | 1:71:A:VAL:HG23 | 40                  | 0.2      | 0.03                | 0.2        |
| (3,814)  | 1:25:A:GLN:H    | 1:71:A:VAL:HG21 | 40                  | 0.2      | 0.03                | 0.2        |
| (3,814)  | 1:25:A:GLN:H    | 1:71:A:VAL:HG22 | 40                  | 0.2      | 0.03                | 0.2        |
| (3,814)  | 1:25:A:GLN:H    | 1:71:A:VAL:HG23 | 40                  | 0.2      | 0.03                | 0.2        |
| (1,737)  | 1:15:A:ARG:H    | 1:14:A:LYS:HA   | 40                  | 0.19     | 0.01                | 0.19       |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H    | 40                  | 0.19     | 0.02                | 0.19       |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H    | 40                  | 0.19     | 0.02                | 0.19       |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H    | 40                  | 0.19     | 0.02                | 0.19       |
| (3,737)  | 1:15:A:ARG:H    | 1:14:A:LYS:HA   | 40                  | 0.19     | 0.01                | 0.19       |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H    | 40                  | 0.19     | 0.02                | 0.19       |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H    | 40                  | 0.19     | 0.02                | 0.19       |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H    | 40                  | 0.19     | 0.02                | 0.19       |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 40                  | 0.19     | 0.03                | 0.19       |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 40                  | 0.19     | 0.03                | 0.19       |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 40                  | 0.19     | 0.03                | 0.19       |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 40                  | 0.19     | 0.03                | 0.19       |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 40                  | 0.19     | 0.03                | 0.19       |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 40                  | 0.19     | 0.03                | 0.19       |
| (1,3004) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG21 | 40                  | 0.19     | 0.04                | 0.19       |
| (1,3004) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG22 | 40                  | 0.19     | 0.04                | 0.19       |
| (1,3004) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG23 | 40                  | 0.19     | 0.04                | 0.19       |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG21 | 40                  | 0.19     | 0.04                | 0.19       |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG22 | 40                  | 0.19     | 0.04                | 0.19       |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG23 | 40                  | 0.19     | 0.04                | 0.19       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1728) | 1:48:A:GLU:HB2  | 1:48:A:GLU:H    | 40                  | 0.19     | 0.01                | 0.19       |
| (3,1731) | 1:48:A:GLU:HB2  | 1:48:A:GLU:H    | 40                  | 0.19     | 0.01                | 0.19       |
| (1,2645) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3   | 40                  | 0.19     | 0.06                | 0.2        |
| (1,650)  | 1:100:A:GLU:H   | 1:99:A:GLY:HA3  | 40                  | 0.19     | 0.04                | 0.21       |
| (1,2278) | 1:96:A:GLU:HG3  | 1:96:A:GLU:HB3  | 40                  | 0.19     | 0.0                 | 0.19       |
| (1,2539) | 1:73:A:PRO:HG2  | 1:73:A:PRO:HA   | 40                  | 0.19     | 0.05                | 0.19       |
| (1,2631) | 1:11:A:GLN:HB3  | 1:11:A:GLN:HG3  | 40                  | 0.19     | 0.0                 | 0.19       |
| (3,650)  | 1:100:A:GLU:H   | 1:99:A:GLY:HA3  | 40                  | 0.19     | 0.04                | 0.21       |
| (3,2281) | 1:96:A:GLU:HG3  | 1:96:A:GLU:HB3  | 40                  | 0.19     | 0.0                 | 0.19       |
| (3,2543) | 1:73:A:PRO:HG2  | 1:73:A:PRO:HA   | 40                  | 0.19     | 0.05                | 0.19       |
| (3,2635) | 1:11:A:GLN:HB3  | 1:11:A:GLN:HG3  | 40                  | 0.19     | 0.0                 | 0.19       |
| (1,2348) | 1:21:A:VAL:HB   | 1:21:A:VAL:HA   | 40                  | 0.19     | 0.01                | 0.19       |
| (3,2351) | 1:21:A:VAL:HB   | 1:21:A:VAL:HA   | 40                  | 0.19     | 0.01                | 0.19       |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H    | 40                  | 0.19     | 0.02                | 0.19       |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H    | 40                  | 0.19     | 0.02                | 0.19       |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H    | 40                  | 0.19     | 0.02                | 0.19       |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H    | 40                  | 0.19     | 0.02                | 0.19       |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H    | 40                  | 0.19     | 0.02                | 0.19       |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H    | 40                  | 0.19     | 0.02                | 0.19       |
| (1,2685) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2   | 40                  | 0.19     | 0.01                | 0.19       |
| (3,2689) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2   | 40                  | 0.19     | 0.01                | 0.19       |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 40                  | 0.19     | 0.03                | 0.18       |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 40                  | 0.19     | 0.03                | 0.18       |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 40                  | 0.19     | 0.03                | 0.18       |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 40                  | 0.19     | 0.03                | 0.18       |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 40                  | 0.19     | 0.03                | 0.18       |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 40                  | 0.19     | 0.03                | 0.18       |
| (1,932)  | 1:98:A:LYS:H    | 1:19:A:ILE:HB   | 40                  | 0.18     | 0.03                | 0.18       |
| (3,933)  | 1:98:A:LYS:H    | 1:19:A:ILE:HB   | 40                  | 0.18     | 0.03                | 0.18       |
| (1,3177) | 1:42:A:TRP:HE1  | 1:81:A:VAL:HB   | 40                  | 0.18     | 0.03                | 0.18       |
| (3,3183) | 1:42:A:TRP:HE1  | 1:81:A:VAL:HB   | 40                  | 0.18     | 0.03                | 0.18       |
| (1,2485) | 1:9:A:PRO:HD2   | 1:9:A:PRO:HB3   | 40                  | 0.18     | 0.03                | 0.18       |
| (3,2488) | 1:9:A:PRO:HD2   | 1:9:A:PRO:HB3   | 40                  | 0.18     | 0.03                | 0.18       |
| (1,871)  | 1:8:A:GLU:H     | 1:9:A:PRO:HD3   | 40                  | 0.18     | 0.02                | 0.18       |
| (3,871)  | 1:8:A:GLU:H     | 1:9:A:PRO:HD3   | 40                  | 0.18     | 0.02                | 0.18       |
| (1,252)  | 1:95:A:ALA:H    | 1:94:A:THR:HG21 | 40                  | 0.18     | 0.03                | 0.19       |
| (1,252)  | 1:95:A:ALA:H    | 1:94:A:THR:HG22 | 40                  | 0.18     | 0.03                | 0.19       |
| (1,252)  | 1:95:A:ALA:H    | 1:94:A:THR:HG23 | 40                  | 0.18     | 0.03                | 0.19       |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 40                  | 0.18     | 0.03                | 0.19       |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 40                  | 0.18     | 0.03                | 0.19       |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 40                  | 0.18     | 0.03                | 0.19       |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 40                  | 0.18     | 0.03                | 0.19       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 40                  | 0.18     | 0.03                | 0.19       |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 40                  | 0.18     | 0.03                | 0.19       |
| (3,252)  | 1:95:A:ALA:H    | 1:94:A:THR:HG21 | 40                  | 0.18     | 0.03                | 0.19       |
| (3,252)  | 1:95:A:ALA:H    | 1:94:A:THR:HG22 | 40                  | 0.18     | 0.03                | 0.19       |
| (3,252)  | 1:95:A:ALA:H    | 1:94:A:THR:HG23 | 40                  | 0.18     | 0.03                | 0.19       |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 40                  | 0.18     | 0.03                | 0.19       |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 40                  | 0.18     | 0.03                | 0.19       |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 40                  | 0.18     | 0.03                | 0.19       |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 40                  | 0.18     | 0.03                | 0.19       |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 40                  | 0.18     | 0.03                | 0.19       |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 40                  | 0.18     | 0.03                | 0.19       |
| (1,801)  | 1:54:A:LYS:H    | 1:54:A:LYS:HD2  | 40                  | 0.18     | 0.02                | 0.18       |
| (3,801)  | 1:54:A:LYS:H    | 1:54:A:LYS:HD2  | 40                  | 0.18     | 0.02                | 0.18       |
| (1,394)  | 1:77:A:GLY:H    | 1:97:A:LEU:HA   | 40                  | 0.18     | 0.03                | 0.18       |
| (3,394)  | 1:77:A:GLY:H    | 1:97:A:LEU:HA   | 40                  | 0.18     | 0.03                | 0.18       |
| (1,1162) | 1:97:A:LEU:H    | 1:29:A:PHE:HE1  | 40                  | 0.18     | 0.03                | 0.17       |
| (1,1162) | 1:97:A:LEU:H    | 1:29:A:PHE:HE2  | 40                  | 0.18     | 0.03                | 0.17       |
| (3,1166) | 1:97:A:LEU:H    | 1:29:A:PHE:HE1  | 40                  | 0.18     | 0.03                | 0.17       |
| (3,1166) | 1:97:A:LEU:H    | 1:29:A:PHE:HE2  | 40                  | 0.18     | 0.03                | 0.17       |
| (1,235)  | 1:13:A:THR:H    | 1:12:A:PHE:HB2  | 40                  | 0.18     | 0.01                | 0.18       |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H    | 40                  | 0.18     | 0.01                | 0.18       |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H    | 40                  | 0.18     | 0.01                | 0.18       |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H    | 40                  | 0.18     | 0.01                | 0.18       |
| (3,235)  | 1:13:A:THR:H    | 1:12:A:PHE:HB2  | 40                  | 0.18     | 0.01                | 0.18       |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H    | 40                  | 0.18     | 0.01                | 0.18       |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H    | 40                  | 0.18     | 0.01                | 0.18       |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H    | 40                  | 0.18     | 0.01                | 0.18       |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA   | 40                  | 0.18     | 0.02                | 0.17       |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA   | 40                  | 0.18     | 0.02                | 0.17       |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA   | 40                  | 0.18     | 0.02                | 0.17       |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA   | 40                  | 0.18     | 0.02                | 0.17       |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA   | 40                  | 0.18     | 0.02                | 0.17       |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA   | 40                  | 0.18     | 0.02                | 0.17       |
| (1,717)  | 1:16:A:ILE:H    | 1:15:A:ARG:HB2  | 40                  | 0.18     | 0.02                | 0.17       |
| (3,717)  | 1:16:A:ILE:H    | 1:15:A:ARG:HB2  | 40                  | 0.18     | 0.02                | 0.17       |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 40                  | 0.18     | 0.01                | 0.17       |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 40                  | 0.18     | 0.01                | 0.17       |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 40                  | 0.18     | 0.01                | 0.17       |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 40                  | 0.18     | 0.01                | 0.17       |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 40                  | 0.18     | 0.01                | 0.17       |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 40                  | 0.18     | 0.01                | 0.17       |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 40                  | 0.17     | 0.03                | 0.18       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 40                  | 0.17     | 0.03                | 0.18       |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 40                  | 0.17     | 0.03                | 0.18       |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 40                  | 0.17     | 0.03                | 0.18       |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 40                  | 0.17     | 0.03                | 0.18       |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 40                  | 0.17     | 0.03                | 0.18       |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 40                  | 0.17     | 0.03                | 0.18       |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 40                  | 0.17     | 0.03                | 0.18       |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 40                  | 0.17     | 0.03                | 0.18       |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 40                  | 0.17     | 0.03                | 0.18       |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 40                  | 0.17     | 0.03                | 0.18       |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 40                  | 0.17     | 0.03                | 0.18       |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 40                  | 0.17     | 0.03                | 0.18       |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 40                  | 0.17     | 0.03                | 0.18       |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 40                  | 0.17     | 0.03                | 0.18       |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 40                  | 0.17     | 0.03                | 0.18       |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 40                  | 0.17     | 0.03                | 0.18       |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 40                  | 0.17     | 0.03                | 0.18       |
| (1,1808) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HE3  | 40                  | 0.17     | 0.0                 | 0.17       |
| (1,2904) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HE3  | 40                  | 0.17     | 0.0                 | 0.17       |
| (1,2907) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD3  | 40                  | 0.17     | 0.0                 | 0.17       |
| (3,1811) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HE3  | 40                  | 0.17     | 0.0                 | 0.17       |
| (3,2911) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HE3  | 40                  | 0.17     | 0.0                 | 0.17       |
| (3,2914) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD3  | 40                  | 0.17     | 0.0                 | 0.17       |
| (1,558)  | 1:47:A:THR:H    | 1:43:A:TYR:HD1  | 40                  | 0.17     | 0.03                | 0.17       |
| (1,558)  | 1:47:A:THR:H    | 1:43:A:TYR:HD2  | 40                  | 0.17     | 0.03                | 0.17       |
| (3,558)  | 1:47:A:THR:H    | 1:43:A:TYR:HD1  | 40                  | 0.17     | 0.03                | 0.17       |
| (3,558)  | 1:47:A:THR:H    | 1:43:A:TYR:HD2  | 40                  | 0.17     | 0.03                | 0.17       |
| (1,49)   | 1:57:A:PHE:H    | 1:56:A:ASN:HB2  | 40                  | 0.17     | 0.02                | 0.18       |
| (3,51)   | 1:57:A:PHE:H    | 1:56:A:ASN:HB2  | 40                  | 0.17     | 0.02                | 0.18       |
| (1,70)   | 1:51:A:GLU:H    | 1:51:A:GLU:HG2  | 40                  | 0.17     | 0.01                | 0.17       |
| (1,1744) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 40                  | 0.17     | 0.01                | 0.17       |
| (3,72)   | 1:51:A:GLU:H    | 1:51:A:GLU:HG2  | 40                  | 0.17     | 0.01                | 0.17       |
| (3,1747) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 40                  | 0.17     | 0.01                | 0.17       |
| (1,605)  | 1:50:A:THR:H    | 1:49:A:LEU:HB2  | 40                  | 0.17     | 0.01                | 0.17       |
| (3,605)  | 1:50:A:THR:H    | 1:49:A:LEU:HB2  | 40                  | 0.17     | 0.01                | 0.17       |
| (1,847)  | 1:83:A:ALA:H    | 1:83:A:ALA:HA   | 40                  | 0.17     | 0.0                 | 0.17       |
| (3,847)  | 1:83:A:ALA:H    | 1:83:A:ALA:HA   | 40                  | 0.17     | 0.0                 | 0.17       |
| (1,3088) | 1:88:A:ARG:HD2  | 1:88:A:ARG:HA   | 40                  | 0.17     | 0.01                | 0.17       |
| (3,3094) | 1:88:A:ARG:HD2  | 1:88:A:ARG:HA   | 40                  | 0.17     | 0.01                | 0.17       |
| (1,57)   | 1:42:A:TRP:H    | 1:41:A:THR:HB   | 40                  | 0.17     | 0.01                | 0.17       |
| (3,59)   | 1:42:A:TRP:H    | 1:41:A:THR:HB   | 40                  | 0.17     | 0.01                | 0.17       |
| (1,531)  | 1:99:A:GLY:H    | 1:98:A:LYS:HG2  | 40                  | 0.17     | 0.02                | 0.17       |

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| Key      | Atom-1          | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (3,531)  | 1:99:A:GLY:H    | 1:98:A:LYS:HG2 | 40                  | 0.17     | 0.02                | 0.17       |
| (1,560)  | 1:47:A:THR:H    | 1:47:A:THR:HA  | 40                  | 0.16     | 0.01                | 0.17       |
| (3,560)  | 1:47:A:THR:H    | 1:47:A:THR:HA  | 40                  | 0.16     | 0.01                | 0.17       |
| (3,589)  | 1:93:A:SER:H    | 1:92:A:ARG:HG2 | 40                  | 0.16     | 0.03                | 0.16       |
| (1,1853) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 40                  | 0.16     | 0.02                | 0.16       |
| (1,1853) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 40                  | 0.16     | 0.02                | 0.16       |
| (1,1853) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 40                  | 0.16     | 0.02                | 0.16       |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 40                  | 0.16     | 0.02                | 0.16       |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 40                  | 0.16     | 0.02                | 0.16       |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 40                  | 0.16     | 0.02                | 0.16       |
| (1,3125) | 1:55:A:TYR:HD1  | 1:51:A:GLU:HA  | 40                  | 0.16     | 0.02                | 0.16       |
| (1,3125) | 1:55:A:TYR:HD2  | 1:51:A:GLU:HA  | 40                  | 0.16     | 0.02                | 0.16       |
| (1,3126) | 1:55:A:TYR:HD1  | 1:51:A:GLU:HA  | 40                  | 0.16     | 0.02                | 0.16       |
| (1,3126) | 1:55:A:TYR:HD2  | 1:51:A:GLU:HA  | 40                  | 0.16     | 0.02                | 0.16       |
| (3,3131) | 1:55:A:TYR:HD1  | 1:51:A:GLU:HA  | 40                  | 0.16     | 0.02                | 0.16       |
| (3,3131) | 1:55:A:TYR:HD2  | 1:51:A:GLU:HA  | 40                  | 0.16     | 0.02                | 0.16       |
| (3,3132) | 1:55:A:TYR:HD1  | 1:51:A:GLU:HA  | 40                  | 0.16     | 0.02                | 0.16       |
| (3,3132) | 1:55:A:TYR:HD2  | 1:51:A:GLU:HA  | 40                  | 0.16     | 0.02                | 0.16       |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1 | 40                  | 0.16     | 0.03                | 0.16       |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2 | 40                  | 0.16     | 0.03                | 0.16       |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1 | 40                  | 0.16     | 0.03                | 0.16       |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2 | 40                  | 0.16     | 0.03                | 0.16       |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1 | 40                  | 0.16     | 0.03                | 0.16       |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2 | 40                  | 0.16     | 0.03                | 0.16       |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1 | 40                  | 0.16     | 0.03                | 0.16       |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2 | 40                  | 0.16     | 0.03                | 0.16       |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1 | 40                  | 0.16     | 0.03                | 0.16       |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2 | 40                  | 0.16     | 0.03                | 0.16       |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1 | 40                  | 0.16     | 0.03                | 0.16       |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2 | 40                  | 0.16     | 0.03                | 0.16       |
| (1,18)   | 1:89:A:GLY:H    | 1:89:A:GLY:HA3 | 40                  | 0.16     | 0.0                 | 0.16       |
| (3,18)   | 1:89:A:GLY:H    | 1:89:A:GLY:HA3 | 40                  | 0.16     | 0.0                 | 0.16       |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA  | 40                  | 0.16     | 0.01                | 0.16       |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA  | 40                  | 0.16     | 0.01                | 0.16       |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA  | 40                  | 0.16     | 0.01                | 0.16       |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA  | 40                  | 0.16     | 0.01                | 0.16       |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA  | 40                  | 0.16     | 0.01                | 0.16       |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA  | 40                  | 0.16     | 0.01                | 0.16       |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA  | 40                  | 0.16     | 0.02                | 0.15       |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA  | 40                  | 0.16     | 0.02                | 0.15       |
| (1,1810) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 40                  | 0.16     | 0.01                | 0.16       |
| (3,1813) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 40                  | 0.16     | 0.01                | 0.16       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1095) | 1:74:A:ASP:H    | 1:73:A:PRO:HA   | 40                  | 0.15     | 0.02                | 0.16       |
| (3,1096) | 1:74:A:ASP:H    | 1:73:A:PRO:HA   | 40                  | 0.15     | 0.02                | 0.16       |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H    | 40                  | 0.15     | 0.01                | 0.15       |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H    | 40                  | 0.15     | 0.01                | 0.15       |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H    | 40                  | 0.15     | 0.01                | 0.15       |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H    | 40                  | 0.15     | 0.01                | 0.15       |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H    | 40                  | 0.15     | 0.01                | 0.15       |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H    | 40                  | 0.15     | 0.01                | 0.15       |
| (1,2474) | 1:4:A:PRO:HG2   | 1:4:A:PRO:HG3   | 40                  | 0.15     | 0.0                 | 0.15       |
| (1,2475) | 1:4:A:PRO:HG3   | 1:4:A:PRO:HG2   | 40                  | 0.15     | 0.0                 | 0.15       |
| (3,2477) | 1:4:A:PRO:HG2   | 1:4:A:PRO:HG3   | 40                  | 0.15     | 0.0                 | 0.15       |
| (3,2478) | 1:4:A:PRO:HG3   | 1:4:A:PRO:HG2   | 40                  | 0.15     | 0.0                 | 0.15       |
| (1,512)  | 1:67:A:THR:H    | 1:66:A:MET:HB2  | 40                  | 0.15     | 0.03                | 0.16       |
| (3,512)  | 1:67:A:THR:H    | 1:66:A:MET:HB2  | 40                  | 0.15     | 0.03                | 0.16       |
| (1,403)  | 1:77:A:GLY:H    | 1:76:A:GLU:HB2  | 40                  | 0.15     | 0.01                | 0.15       |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H    | 40                  | 0.15     | 0.01                | 0.15       |
| (3,403)  | 1:77:A:GLY:H    | 1:76:A:GLU:HB2  | 40                  | 0.15     | 0.01                | 0.15       |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H    | 40                  | 0.15     | 0.01                | 0.15       |
| (1,1401) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H    | 40                  | 0.15     | 0.02                | 0.15       |
| (1,1401) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H    | 40                  | 0.15     | 0.02                | 0.15       |
| (1,1401) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H    | 40                  | 0.15     | 0.02                | 0.15       |
| (3,1405) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H    | 40                  | 0.15     | 0.02                | 0.15       |
| (3,1405) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H    | 40                  | 0.15     | 0.02                | 0.15       |
| (3,1405) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H    | 40                  | 0.15     | 0.02                | 0.15       |
| (1,2859) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 40                  | 0.15     | 0.01                | 0.15       |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 40                  | 0.15     | 0.01                | 0.15       |
| (1,373)  | 1:97:A:LEU:H    | 1:97:A:LEU:HD11 | 40                  | 0.15     | 0.01                | 0.15       |
| (1,373)  | 1:97:A:LEU:H    | 1:97:A:LEU:HD12 | 40                  | 0.15     | 0.01                | 0.15       |
| (1,373)  | 1:97:A:LEU:H    | 1:97:A:LEU:HD13 | 40                  | 0.15     | 0.01                | 0.15       |
| (3,373)  | 1:97:A:LEU:H    | 1:97:A:LEU:HD11 | 40                  | 0.15     | 0.01                | 0.15       |
| (3,373)  | 1:97:A:LEU:H    | 1:97:A:LEU:HD12 | 40                  | 0.15     | 0.01                | 0.15       |
| (3,373)  | 1:97:A:LEU:H    | 1:97:A:LEU:HD13 | 40                  | 0.15     | 0.01                | 0.15       |
| (1,1514) | 1:66:A:MET:HE1  | 1:66:A:MET:H    | 40                  | 0.14     | 0.01                | 0.15       |
| (1,1514) | 1:66:A:MET:HE2  | 1:66:A:MET:H    | 40                  | 0.14     | 0.01                | 0.15       |
| (1,1514) | 1:66:A:MET:HE3  | 1:66:A:MET:H    | 40                  | 0.14     | 0.01                | 0.15       |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H    | 40                  | 0.14     | 0.01                | 0.15       |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H    | 40                  | 0.14     | 0.01                | 0.15       |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H    | 40                  | 0.14     | 0.01                | 0.15       |
| (1,528)  | 1:99:A:GLY:H    | 1:98:A:LYS:HB2  | 40                  | 0.14     | 0.02                | 0.15       |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 40                  | 0.14     | 0.02                | 0.14       |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 40                  | 0.14     | 0.02                | 0.14       |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 40                  | 0.14     | 0.02                | 0.14       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (3,528)  | 1:99:A:GLY:H    | 1:98:A:LYS:HB2  | 40                  | 0.14     | 0.02                | 0.15       |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 40                  | 0.14     | 0.02                | 0.14       |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 40                  | 0.14     | 0.02                | 0.14       |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 40                  | 0.14     | 0.02                | 0.14       |
| (1,2903) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 40                  | 0.14     | 0.01                | 0.14       |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 40                  | 0.14     | 0.01                | 0.14       |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1  | 40                  | 0.14     | 0.02                | 0.14       |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2  | 40                  | 0.14     | 0.02                | 0.14       |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1  | 40                  | 0.14     | 0.02                | 0.14       |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2  | 40                  | 0.14     | 0.02                | 0.14       |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1  | 40                  | 0.14     | 0.02                | 0.14       |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2  | 40                  | 0.14     | 0.02                | 0.14       |
| (1,3118) | 1:55:A:TYR:HD1  | 1:68:A:ILE:HG21 | 40                  | 0.14     | 0.02                | 0.14       |
| (1,3118) | 1:55:A:TYR:HD1  | 1:68:A:ILE:HG22 | 40                  | 0.14     | 0.02                | 0.14       |
| (1,3118) | 1:55:A:TYR:HD1  | 1:68:A:ILE:HG23 | 40                  | 0.14     | 0.02                | 0.14       |
| (1,3118) | 1:55:A:TYR:HD2  | 1:68:A:ILE:HG21 | 40                  | 0.14     | 0.02                | 0.14       |
| (1,3118) | 1:55:A:TYR:HD2  | 1:68:A:ILE:HG22 | 40                  | 0.14     | 0.02                | 0.14       |
| (1,3118) | 1:55:A:TYR:HD2  | 1:68:A:ILE:HG23 | 40                  | 0.14     | 0.02                | 0.14       |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1  | 40                  | 0.14     | 0.02                | 0.14       |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2  | 40                  | 0.14     | 0.02                | 0.14       |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1  | 40                  | 0.14     | 0.02                | 0.14       |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2  | 40                  | 0.14     | 0.02                | 0.14       |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1  | 40                  | 0.14     | 0.02                | 0.14       |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2  | 40                  | 0.14     | 0.02                | 0.14       |
| (3,3124) | 1:55:A:TYR:HD1  | 1:68:A:ILE:HG21 | 40                  | 0.14     | 0.02                | 0.14       |
| (3,3124) | 1:55:A:TYR:HD1  | 1:68:A:ILE:HG22 | 40                  | 0.14     | 0.02                | 0.14       |
| (3,3124) | 1:55:A:TYR:HD1  | 1:68:A:ILE:HG23 | 40                  | 0.14     | 0.02                | 0.14       |
| (3,3124) | 1:55:A:TYR:HD2  | 1:68:A:ILE:HG21 | 40                  | 0.14     | 0.02                | 0.14       |
| (3,3124) | 1:55:A:TYR:HD2  | 1:68:A:ILE:HG22 | 40                  | 0.14     | 0.02                | 0.14       |
| (3,3124) | 1:55:A:TYR:HD2  | 1:68:A:ILE:HG23 | 40                  | 0.14     | 0.02                | 0.14       |
| (1,1400) | 1:95:A:ALA:HB1  | 1:16:A:ILE:HG12 | 40                  | 0.14     | 0.01                | 0.14       |
| (1,1400) | 1:95:A:ALA:HB2  | 1:16:A:ILE:HG12 | 40                  | 0.14     | 0.01                | 0.14       |
| (1,1400) | 1:95:A:ALA:HB3  | 1:16:A:ILE:HG12 | 40                  | 0.14     | 0.01                | 0.14       |
| (3,1404) | 1:95:A:ALA:HB1  | 1:16:A:ILE:HG12 | 40                  | 0.14     | 0.01                | 0.14       |
| (3,1404) | 1:95:A:ALA:HB2  | 1:16:A:ILE:HG12 | 40                  | 0.14     | 0.01                | 0.14       |
| (3,1404) | 1:95:A:ALA:HB3  | 1:16:A:ILE:HG12 | 40                  | 0.14     | 0.01                | 0.14       |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 40                  | 0.14     | 0.03                | 0.13       |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 40                  | 0.14     | 0.03                | 0.13       |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 40                  | 0.14     | 0.03                | 0.13       |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 40                  | 0.14     | 0.03                | 0.13       |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 40                  | 0.14     | 0.03                | 0.13       |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 40                  | 0.14     | 0.03                | 0.13       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,48)   | 1:57:A:PHE:H    | 1:57:A:PHE:HB3  | 40                  | 0.14     | 0.01                | 0.14       |
| (3,50)   | 1:57:A:PHE:H    | 1:57:A:PHE:HB3  | 40                  | 0.14     | 0.01                | 0.14       |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 40                  | 0.14     | 0.01                | 0.14       |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 40                  | 0.14     | 0.01                | 0.14       |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 40                  | 0.14     | 0.01                | 0.14       |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 40                  | 0.14     | 0.01                | 0.14       |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 40                  | 0.14     | 0.01                | 0.14       |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 40                  | 0.14     | 0.01                | 0.14       |
| (1,1811) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2  | 40                  | 0.14     | 0.01                | 0.14       |
| (3,1814) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2  | 40                  | 0.14     | 0.01                | 0.14       |
| (1,296)  | 1:31:A:CYS:H    | 1:30:A:GLU:HB3  | 40                  | 0.14     | 0.02                | 0.14       |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 40                  | 0.14     | 0.02                | 0.14       |
| (3,296)  | 1:31:A:CYS:H    | 1:30:A:GLU:HB3  | 40                  | 0.14     | 0.02                | 0.14       |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 40                  | 0.14     | 0.02                | 0.14       |
| (1,978)  | 1:20:A:VAL:H    | 1:19:A:ILE:HB   | 40                  | 0.14     | 0.01                | 0.14       |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 40                  | 0.14     | 0.01                | 0.14       |
| (3,979)  | 1:20:A:VAL:H    | 1:19:A:ILE:HB   | 40                  | 0.14     | 0.01                | 0.14       |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 40                  | 0.14     | 0.01                | 0.14       |
| (1,809)  | 1:78:A:VAL:H    | 1:78:A:VAL:HG11 | 40                  | 0.14     | 0.01                | 0.13       |
| (1,809)  | 1:78:A:VAL:H    | 1:78:A:VAL:HG12 | 40                  | 0.14     | 0.01                | 0.13       |
| (1,809)  | 1:78:A:VAL:H    | 1:78:A:VAL:HG13 | 40                  | 0.14     | 0.01                | 0.13       |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H    | 40                  | 0.14     | 0.01                | 0.13       |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H    | 40                  | 0.14     | 0.01                | 0.13       |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H    | 40                  | 0.14     | 0.01                | 0.13       |
| (3,809)  | 1:78:A:VAL:H    | 1:78:A:VAL:HG11 | 40                  | 0.14     | 0.01                | 0.13       |
| (3,809)  | 1:78:A:VAL:H    | 1:78:A:VAL:HG12 | 40                  | 0.14     | 0.01                | 0.13       |
| (3,809)  | 1:78:A:VAL:H    | 1:78:A:VAL:HG13 | 40                  | 0.14     | 0.01                | 0.13       |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H    | 40                  | 0.14     | 0.01                | 0.13       |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H    | 40                  | 0.14     | 0.01                | 0.13       |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H    | 40                  | 0.14     | 0.01                | 0.13       |
| (1,1084) | 1:99:A:GLY:H    | 1:99:A:GLY:HA2  | 40                  | 0.13     | 0.0                 | 0.13       |
| (3,1085) | 1:99:A:GLY:H    | 1:99:A:GLY:HA2  | 40                  | 0.13     | 0.0                 | 0.13       |
| (1,2491) | 1:9:A:PRO:HB2   | 1:9:A:PRO:HA    | 40                  | 0.13     | 0.02                | 0.14       |
| (3,2494) | 1:9:A:PRO:HB2   | 1:9:A:PRO:HA    | 40                  | 0.13     | 0.02                | 0.14       |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 40                  | 0.13     | 0.0                 | 0.13       |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 40                  | 0.13     | 0.0                 | 0.13       |
| (1,567)  | 1:47:A:THR:H    | 1:47:A:THR:HG21 | 40                  | 0.13     | 0.01                | 0.13       |
| (1,567)  | 1:47:A:THR:H    | 1:47:A:THR:HG22 | 40                  | 0.13     | 0.01                | 0.13       |
| (1,567)  | 1:47:A:THR:H    | 1:47:A:THR:HG23 | 40                  | 0.13     | 0.01                | 0.13       |
| (3,567)  | 1:47:A:THR:H    | 1:47:A:THR:HG21 | 40                  | 0.13     | 0.01                | 0.13       |
| (3,567)  | 1:47:A:THR:H    | 1:47:A:THR:HG22 | 40                  | 0.13     | 0.01                | 0.13       |
| (3,567)  | 1:47:A:THR:H    | 1:47:A:THR:HG23 | 40                  | 0.13     | 0.01                | 0.13       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1269) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 40                  | 0.13     | 0.0                 | 0.13       |
| (1,1270) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3   | 40                  | 0.13     | 0.0                 | 0.13       |
| (1,2150) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 40                  | 0.13     | 0.0                 | 0.13       |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 40                  | 0.13     | 0.0                 | 0.13       |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3   | 40                  | 0.13     | 0.0                 | 0.13       |
| (3,2153) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 40                  | 0.13     | 0.0                 | 0.13       |
| (1,1803) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HB3  | 40                  | 0.13     | 0.0                 | 0.13       |
| (1,2953) | 1:98:A:LYS:HB3  | 1:98:A:LYS:HG2  | 40                  | 0.13     | 0.0                 | 0.13       |
| (3,1806) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HB3  | 40                  | 0.13     | 0.0                 | 0.13       |
| (3,2961) | 1:98:A:LYS:HB3  | 1:98:A:LYS:HG2  | 40                  | 0.13     | 0.0                 | 0.13       |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 40                  | 0.12     | 0.0                 | 0.12       |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 40                  | 0.12     | 0.0                 | 0.12       |
| (1,2713) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 40                  | 0.12     | 0.0                 | 0.12       |
| (3,2717) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 40                  | 0.12     | 0.0                 | 0.12       |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA   | 40                  | 0.12     | 0.0                 | 0.12       |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA   | 40                  | 0.12     | 0.0                 | 0.12       |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA   | 40                  | 0.12     | 0.0                 | 0.12       |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA   | 40                  | 0.12     | 0.0                 | 0.12       |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA   | 40                  | 0.12     | 0.0                 | 0.12       |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA   | 40                  | 0.12     | 0.0                 | 0.12       |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 40                  | 0.11     | 0.0                 | 0.11       |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 40                  | 0.11     | 0.0                 | 0.11       |
| (1,3212) | 1:65:A:TYR:HE1  | 1:58:A:ARG:HB3  | 39                  | 0.23     | 0.05                | 0.23       |
| (1,3212) | 1:65:A:TYR:HE2  | 1:58:A:ARG:HB3  | 39                  | 0.23     | 0.05                | 0.23       |
| (3,3218) | 1:65:A:TYR:HE1  | 1:58:A:ARG:HB3  | 39                  | 0.23     | 0.05                | 0.23       |
| (3,3218) | 1:65:A:TYR:HE2  | 1:58:A:ARG:HB3  | 39                  | 0.23     | 0.05                | 0.23       |
| (1,546)  | 1:71:A:VAL:H    | 1:24:A:HIS:HA   | 39                  | 0.22     | 0.05                | 0.22       |
| (3,546)  | 1:71:A:VAL:H    | 1:24:A:HIS:HA   | 39                  | 0.22     | 0.05                | 0.22       |
| (1,870)  | 1:8:A:GLU:H     | 1:9:A:PRO:HD2   | 39                  | 0.19     | 0.03                | 0.19       |
| (3,870)  | 1:8:A:GLU:H     | 1:9:A:PRO:HD2   | 39                  | 0.19     | 0.03                | 0.19       |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 39                  | 0.19     | 0.04                | 0.19       |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 39                  | 0.19     | 0.04                | 0.19       |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 39                  | 0.19     | 0.04                | 0.19       |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 39                  | 0.19     | 0.04                | 0.19       |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 39                  | 0.19     | 0.04                | 0.19       |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 39                  | 0.19     | 0.04                | 0.19       |
| (1,139)  | 1:101:A:LEU:H   | 1:100:A:GLU:H   | 39                  | 0.18     | 0.02                | 0.19       |
| (1,1137) | 1:100:A:GLU:H   | 1:101:A:LEU:H   | 39                  | 0.18     | 0.02                | 0.19       |
| (3,141)  | 1:101:A:LEU:H   | 1:100:A:GLU:H   | 39                  | 0.18     | 0.02                | 0.19       |
| (3,1140) | 1:100:A:GLU:H   | 1:101:A:LEU:H   | 39                  | 0.18     | 0.02                | 0.19       |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 39                  | 0.16     | 0.02                | 0.16       |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 39                  | 0.16     | 0.02                | 0.16       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 39                  | 0.16     | 0.02                | 0.16       |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 39                  | 0.16     | 0.02                | 0.16       |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 39                  | 0.16     | 0.02                | 0.16       |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 39                  | 0.16     | 0.02                | 0.16       |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 39                  | 0.16     | 0.03                | 0.16       |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 39                  | 0.16     | 0.03                | 0.16       |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 39                  | 0.16     | 0.03                | 0.15       |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 39                  | 0.16     | 0.03                | 0.15       |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 39                  | 0.16     | 0.03                | 0.15       |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 39                  | 0.16     | 0.03                | 0.15       |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 39                  | 0.16     | 0.03                | 0.15       |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 39                  | 0.16     | 0.03                | 0.15       |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 39                  | 0.16     | 0.03                | 0.15       |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 39                  | 0.16     | 0.03                | 0.15       |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 39                  | 0.16     | 0.03                | 0.15       |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 39                  | 0.16     | 0.03                | 0.15       |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 39                  | 0.16     | 0.03                | 0.15       |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 39                  | 0.16     | 0.03                | 0.15       |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 39                  | 0.15     | 0.02                | 0.16       |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 39                  | 0.15     | 0.02                | 0.16       |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 39                  | 0.15     | 0.02                | 0.16       |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 39                  | 0.15     | 0.02                | 0.16       |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 39                  | 0.15     | 0.02                | 0.16       |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 39                  | 0.15     | 0.02                | 0.16       |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 39                  | 0.15     | 0.02                | 0.16       |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 39                  | 0.15     | 0.02                | 0.16       |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 39                  | 0.15     | 0.02                | 0.16       |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 39                  | 0.15     | 0.02                | 0.16       |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 39                  | 0.15     | 0.02                | 0.16       |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 39                  | 0.15     | 0.02                | 0.16       |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 39                  | 0.15     | 0.02                | 0.16       |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 39                  | 0.15     | 0.02                | 0.16       |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 39                  | 0.15     | 0.02                | 0.16       |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 39                  | 0.15     | 0.02                | 0.16       |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 39                  | 0.15     | 0.02                | 0.16       |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 39                  | 0.15     | 0.02                | 0.16       |
| (1,2675) | 1:25:A:GLN:HG3  | 1:26:A:SER:H    | 39                  | 0.15     | 0.02                | 0.15       |
| (3,2679) | 1:25:A:GLN:HG3  | 1:26:A:SER:H    | 39                  | 0.15     | 0.02                | 0.15       |
| (1,370)  | 1:18:A:ASN:H    | 1:95:A:ALA:HB1  | 39                  | 0.14     | 0.02                | 0.15       |
| (1,370)  | 1:18:A:ASN:H    | 1:95:A:ALA:HB2  | 39                  | 0.14     | 0.02                | 0.15       |
| (1,370)  | 1:18:A:ASN:H    | 1:95:A:ALA:HB3  | 39                  | 0.14     | 0.02                | 0.15       |
| (1,1403) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H    | 39                  | 0.14     | 0.02                | 0.15       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1403) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H    | 39                  | 0.14     | 0.02                | 0.15       |
| (1,1403) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H    | 39                  | 0.14     | 0.02                | 0.15       |
| (3,370)  | 1:18:A:ASN:H    | 1:95:A:ALA:HB1  | 39                  | 0.14     | 0.02                | 0.15       |
| (3,370)  | 1:18:A:ASN:H    | 1:95:A:ALA:HB2  | 39                  | 0.14     | 0.02                | 0.15       |
| (3,370)  | 1:18:A:ASN:H    | 1:95:A:ALA:HB3  | 39                  | 0.14     | 0.02                | 0.15       |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H    | 39                  | 0.14     | 0.02                | 0.15       |
| (3,1407) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H    | 39                  | 0.14     | 0.02                | 0.15       |
| (3,1407) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H    | 39                  | 0.14     | 0.02                | 0.15       |
| (1,2287) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 39                  | 0.14     | 0.01                | 0.14       |
| (3,2290) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 39                  | 0.14     | 0.01                | 0.14       |
| (1,2686) | 1:8:A:GLU:HB3   | 1:8:A:GLU:HG2   | 39                  | 0.14     | 0.02                | 0.14       |
| (3,2690) | 1:8:A:GLU:HB3   | 1:8:A:GLU:HG2   | 39                  | 0.14     | 0.02                | 0.14       |
| (1,3084) | 1:98:A:LYS:HD3  | 1:20:A:VAL:HG21 | 39                  | 0.14     | 0.03                | 0.13       |
| (1,3084) | 1:98:A:LYS:HD3  | 1:20:A:VAL:HG22 | 39                  | 0.14     | 0.03                | 0.13       |
| (1,3084) | 1:98:A:LYS:HD3  | 1:20:A:VAL:HG23 | 39                  | 0.14     | 0.03                | 0.13       |
| (3,3090) | 1:98:A:LYS:HD3  | 1:20:A:VAL:HG21 | 39                  | 0.14     | 0.03                | 0.13       |
| (3,3090) | 1:98:A:LYS:HD3  | 1:20:A:VAL:HG22 | 39                  | 0.14     | 0.03                | 0.13       |
| (3,3090) | 1:98:A:LYS:HD3  | 1:20:A:VAL:HG23 | 39                  | 0.14     | 0.03                | 0.13       |
| (1,3209) | 1:57:A:PHE:HZ   | 1:55:A:TYR:HD1  | 39                  | 0.14     | 0.03                | 0.12       |
| (1,3209) | 1:57:A:PHE:HZ   | 1:55:A:TYR:HD2  | 39                  | 0.14     | 0.03                | 0.12       |
| (3,3215) | 1:57:A:PHE:HZ   | 1:55:A:TYR:HD1  | 39                  | 0.14     | 0.03                | 0.12       |
| (3,3215) | 1:57:A:PHE:HZ   | 1:55:A:TYR:HD2  | 39                  | 0.14     | 0.03                | 0.12       |
| (1,653)  | 1:100:A:GLU:H   | 1:100:A:GLU:HG2 | 39                  | 0.13     | 0.02                | 0.13       |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 39                  | 0.13     | 0.02                | 0.13       |
| (3,653)  | 1:100:A:GLU:H   | 1:100:A:GLU:HG2 | 39                  | 0.13     | 0.02                | 0.13       |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 39                  | 0.13     | 0.02                | 0.13       |
| (1,2498) | 1:9:A:PRO:HG3   | 1:9:A:PRO:HB2   | 39                  | 0.13     | 0.02                | 0.14       |
| (3,2501) | 1:9:A:PRO:HG3   | 1:9:A:PRO:HB2   | 39                  | 0.13     | 0.02                | 0.14       |
| (1,2949) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 39                  | 0.13     | 0.01                | 0.13       |
| (3,2957) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 39                  | 0.13     | 0.01                | 0.13       |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 39                  | 0.12     | 0.01                | 0.12       |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 39                  | 0.12     | 0.01                | 0.12       |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 39                  | 0.12     | 0.01                | 0.12       |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 39                  | 0.12     | 0.01                | 0.12       |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 39                  | 0.12     | 0.01                | 0.12       |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 39                  | 0.12     | 0.01                | 0.12       |
| (1,2679) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HG2  | 39                  | 0.12     | 0.0                 | 0.12       |
| (3,2683) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HG2  | 39                  | 0.12     | 0.0                 | 0.12       |
| (1,239)  | 1:13:A:THR:H    | 1:14:A:LYS:HA   | 39                  | 0.12     | 0.01                | 0.12       |
| (3,239)  | 1:13:A:THR:H    | 1:14:A:LYS:HA   | 39                  | 0.12     | 0.01                | 0.12       |
| (1,2918) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 38                  | 0.25     | 0.04                | 0.26       |
| (3,2925) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 38                  | 0.25     | 0.04                | 0.26       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,918)  | 1:37:A:ASP:H    | 1:36:A:ASP:HB3  | 38                  | 0.23     | 0.05                | 0.22       |
| (1,2597) | 1:36:A:ASP:HB3  | 1:37:A:ASP:H    | 38                  | 0.23     | 0.05                | 0.22       |
| (3,919)  | 1:37:A:ASP:H    | 1:36:A:ASP:HB3  | 38                  | 0.23     | 0.05                | 0.22       |
| (3,2601) | 1:36:A:ASP:HB3  | 1:37:A:ASP:H    | 38                  | 0.23     | 0.05                | 0.22       |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 38                  | 0.21     | 0.01                | 0.21       |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 38                  | 0.21     | 0.01                | 0.21       |
| (1,869)  | 1:8:A:GLU:H     | 1:7:A:ALA:HA    | 38                  | 0.2      | 0.04                | 0.19       |
| (3,869)  | 1:8:A:GLU:H     | 1:7:A:ALA:HA    | 38                  | 0.2      | 0.04                | 0.19       |
| (1,1163) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 38                  | 0.2      | 0.03                | 0.2        |
| (3,1167) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 38                  | 0.2      | 0.03                | 0.2        |
| (1,3200) | 1:55:A:TYR:HD1  | 1:49:A:LEU:HD21 | 38                  | 0.15     | 0.03                | 0.15       |
| (1,3200) | 1:55:A:TYR:HD1  | 1:49:A:LEU:HD22 | 38                  | 0.15     | 0.03                | 0.15       |
| (1,3200) | 1:55:A:TYR:HD1  | 1:49:A:LEU:HD23 | 38                  | 0.15     | 0.03                | 0.15       |
| (1,3200) | 1:55:A:TYR:HD2  | 1:49:A:LEU:HD21 | 38                  | 0.15     | 0.03                | 0.15       |
| (1,3200) | 1:55:A:TYR:HD2  | 1:49:A:LEU:HD22 | 38                  | 0.15     | 0.03                | 0.15       |
| (1,3200) | 1:55:A:TYR:HD2  | 1:49:A:LEU:HD23 | 38                  | 0.15     | 0.03                | 0.15       |
| (3,3206) | 1:55:A:TYR:HD1  | 1:49:A:LEU:HD21 | 38                  | 0.15     | 0.03                | 0.15       |
| (3,3206) | 1:55:A:TYR:HD1  | 1:49:A:LEU:HD22 | 38                  | 0.15     | 0.03                | 0.15       |
| (3,3206) | 1:55:A:TYR:HD1  | 1:49:A:LEU:HD23 | 38                  | 0.15     | 0.03                | 0.15       |
| (3,3206) | 1:55:A:TYR:HD2  | 1:49:A:LEU:HD21 | 38                  | 0.15     | 0.03                | 0.15       |
| (3,3206) | 1:55:A:TYR:HD2  | 1:49:A:LEU:HD22 | 38                  | 0.15     | 0.03                | 0.15       |
| (3,3206) | 1:55:A:TYR:HD2  | 1:49:A:LEU:HD23 | 38                  | 0.15     | 0.03                | 0.15       |
| (1,2409) | 1:10:A:ILE:HA   | 1:11:A:GLN:HG2  | 38                  | 0.15     | 0.01                | 0.15       |
| (3,2412) | 1:10:A:ILE:HA   | 1:11:A:GLN:HG2  | 38                  | 0.15     | 0.01                | 0.15       |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 38                  | 0.14     | 0.02                | 0.15       |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 38                  | 0.14     | 0.02                | 0.15       |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 38                  | 0.14     | 0.02                | 0.15       |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 38                  | 0.14     | 0.02                | 0.15       |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 38                  | 0.14     | 0.02                | 0.15       |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 38                  | 0.14     | 0.02                | 0.15       |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 38                  | 0.14     | 0.02                | 0.15       |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 38                  | 0.14     | 0.02                | 0.15       |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 38                  | 0.14     | 0.02                | 0.15       |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 38                  | 0.14     | 0.02                | 0.15       |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 38                  | 0.14     | 0.02                | 0.15       |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 38                  | 0.14     | 0.02                | 0.15       |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 38                  | 0.14     | 0.02                | 0.15       |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 38                  | 0.14     | 0.02                | 0.15       |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 38                  | 0.14     | 0.02                | 0.15       |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 38                  | 0.14     | 0.02                | 0.15       |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 38                  | 0.14     | 0.02                | 0.15       |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 38                  | 0.14     | 0.02                | 0.15       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,967)  | 1:21:A:VAL:H    | 1:99:A:GLY:HA3  | 38                  | 0.14     | 0.02                | 0.13       |
| (3,968)  | 1:21:A:VAL:H    | 1:99:A:GLY:HA3  | 38                  | 0.14     | 0.02                | 0.13       |
| (1,551)  | 1:71:A:VAL:H    | 1:71:A:VAL:HG11 | 38                  | 0.11     | 0.01                | 0.11       |
| (1,551)  | 1:71:A:VAL:H    | 1:71:A:VAL:HG12 | 38                  | 0.11     | 0.01                | 0.11       |
| (1,551)  | 1:71:A:VAL:H    | 1:71:A:VAL:HG13 | 38                  | 0.11     | 0.01                | 0.11       |
| (3,551)  | 1:71:A:VAL:H    | 1:71:A:VAL:HG11 | 38                  | 0.11     | 0.01                | 0.11       |
| (3,551)  | 1:71:A:VAL:H    | 1:71:A:VAL:HG12 | 38                  | 0.11     | 0.01                | 0.11       |
| (3,551)  | 1:71:A:VAL:H    | 1:71:A:VAL:HG13 | 38                  | 0.11     | 0.01                | 0.11       |
| (1,2968) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 37                  | 0.22     | 0.0                 | 0.22       |
| (3,2976) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 37                  | 0.22     | 0.0                 | 0.22       |
| (1,849)  | 1:83:A:ALA:H    | 1:91:A:ALA:HB1  | 37                  | 0.17     | 0.04                | 0.15       |
| (1,849)  | 1:83:A:ALA:H    | 1:91:A:ALA:HB2  | 37                  | 0.17     | 0.04                | 0.15       |
| (1,849)  | 1:83:A:ALA:H    | 1:91:A:ALA:HB3  | 37                  | 0.17     | 0.04                | 0.15       |
| (3,849)  | 1:83:A:ALA:H    | 1:91:A:ALA:HB1  | 37                  | 0.17     | 0.04                | 0.15       |
| (3,849)  | 1:83:A:ALA:H    | 1:91:A:ALA:HB2  | 37                  | 0.17     | 0.04                | 0.15       |
| (3,849)  | 1:83:A:ALA:H    | 1:91:A:ALA:HB3  | 37                  | 0.17     | 0.04                | 0.15       |
| (1,2754) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 37                  | 0.16     | 0.04                | 0.16       |
| (3,2761) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 37                  | 0.16     | 0.04                | 0.16       |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 37                  | 0.14     | 0.02                | 0.14       |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 37                  | 0.14     | 0.02                | 0.14       |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 37                  | 0.14     | 0.02                | 0.14       |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 37                  | 0.14     | 0.02                | 0.14       |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 37                  | 0.14     | 0.02                | 0.14       |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 37                  | 0.14     | 0.02                | 0.14       |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 37                  | 0.14     | 0.02                | 0.14       |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 37                  | 0.14     | 0.02                | 0.14       |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 37                  | 0.14     | 0.02                | 0.14       |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 37                  | 0.14     | 0.02                | 0.14       |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 37                  | 0.14     | 0.02                | 0.14       |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 37                  | 0.14     | 0.02                | 0.14       |
| (1,201)  | 1:90:A:GLU:H    | 1:89:A:GLY:HA2  | 37                  | 0.14     | 0.02                | 0.13       |
| (3,201)  | 1:90:A:GLU:H    | 1:89:A:GLY:HA2  | 37                  | 0.14     | 0.02                | 0.13       |
| (1,1052) | 1:26:A:SER:H    | 1:25:A:GLN:HG2  | 37                  | 0.13     | 0.01                | 0.13       |
| (3,1051) | 1:26:A:SER:H    | 1:25:A:GLN:HG2  | 37                  | 0.13     | 0.01                | 0.13       |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB   | 36                  | 0.21     | 0.0                 | 0.21       |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB   | 36                  | 0.21     | 0.0                 | 0.21       |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB   | 36                  | 0.21     | 0.0                 | 0.21       |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB   | 36                  | 0.21     | 0.0                 | 0.21       |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB   | 36                  | 0.21     | 0.0                 | 0.21       |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB   | 36                  | 0.21     | 0.0                 | 0.21       |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 36                  | 0.2      | 0.06                | 0.22       |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 36                  | 0.2      | 0.06                | 0.22       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 36                  | 0.2      | 0.06                | 0.22       |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 36                  | 0.2      | 0.06                | 0.22       |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 36                  | 0.2      | 0.06                | 0.22       |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 36                  | 0.2      | 0.06                | 0.22       |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1  | 36                  | 0.2      | 0.06                | 0.22       |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2  | 36                  | 0.2      | 0.06                | 0.22       |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1  | 36                  | 0.2      | 0.06                | 0.22       |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2  | 36                  | 0.2      | 0.06                | 0.22       |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1  | 36                  | 0.2      | 0.06                | 0.22       |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2  | 36                  | 0.2      | 0.06                | 0.22       |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1  | 36                  | 0.2      | 0.06                | 0.22       |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2  | 36                  | 0.2      | 0.06                | 0.22       |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1  | 36                  | 0.2      | 0.06                | 0.22       |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2  | 36                  | 0.2      | 0.06                | 0.22       |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1  | 36                  | 0.2      | 0.06                | 0.22       |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2  | 36                  | 0.2      | 0.06                | 0.22       |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 36                  | 0.19     | 0.0                 | 0.19       |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 36                  | 0.19     | 0.0                 | 0.19       |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 36                  | 0.19     | 0.0                 | 0.19       |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 36                  | 0.19     | 0.0                 | 0.19       |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 36                  | 0.19     | 0.0                 | 0.19       |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 36                  | 0.19     | 0.0                 | 0.19       |
| (1,2402) | 1:66:A:MET:HE1  | 1:29:A:PHE:HZ   | 36                  | 0.16     | 0.03                | 0.17       |
| (1,2402) | 1:66:A:MET:HE2  | 1:29:A:PHE:HZ   | 36                  | 0.16     | 0.03                | 0.17       |
| (1,2402) | 1:66:A:MET:HE3  | 1:29:A:PHE:HZ   | 36                  | 0.16     | 0.03                | 0.17       |
| (3,2405) | 1:66:A:MET:HE1  | 1:29:A:PHE:HZ   | 36                  | 0.16     | 0.03                | 0.17       |
| (3,2405) | 1:66:A:MET:HE2  | 1:29:A:PHE:HZ   | 36                  | 0.16     | 0.03                | 0.17       |
| (3,2405) | 1:66:A:MET:HE3  | 1:29:A:PHE:HZ   | 36                  | 0.16     | 0.03                | 0.17       |
| (1,529)  | 1:99:A:GLY:H    | 1:76:A:GLU:HB2  | 36                  | 0.16     | 0.03                | 0.16       |
| (3,529)  | 1:99:A:GLY:H    | 1:76:A:GLU:HB2  | 36                  | 0.16     | 0.03                | 0.16       |
| (1,3092) | 1:66:A:MET:HE1  | 1:55:A:TYR:HE1  | 36                  | 0.14     | 0.02                | 0.14       |
| (1,3092) | 1:66:A:MET:HE1  | 1:55:A:TYR:HE2  | 36                  | 0.14     | 0.02                | 0.14       |
| (1,3092) | 1:66:A:MET:HE2  | 1:55:A:TYR:HE1  | 36                  | 0.14     | 0.02                | 0.14       |
| (1,3092) | 1:66:A:MET:HE2  | 1:55:A:TYR:HE2  | 36                  | 0.14     | 0.02                | 0.14       |
| (1,3092) | 1:66:A:MET:HE3  | 1:55:A:TYR:HE1  | 36                  | 0.14     | 0.02                | 0.14       |
| (1,3092) | 1:66:A:MET:HE3  | 1:55:A:TYR:HE2  | 36                  | 0.14     | 0.02                | 0.14       |
| (3,3098) | 1:66:A:MET:HE1  | 1:55:A:TYR:HE1  | 36                  | 0.14     | 0.02                | 0.14       |
| (3,3098) | 1:66:A:MET:HE1  | 1:55:A:TYR:HE2  | 36                  | 0.14     | 0.02                | 0.14       |
| (3,3098) | 1:66:A:MET:HE2  | 1:55:A:TYR:HE1  | 36                  | 0.14     | 0.02                | 0.14       |
| (3,3098) | 1:66:A:MET:HE2  | 1:55:A:TYR:HE2  | 36                  | 0.14     | 0.02                | 0.14       |
| (3,3098) | 1:66:A:MET:HE3  | 1:55:A:TYR:HE1  | 36                  | 0.14     | 0.02                | 0.14       |
| (3,3098) | 1:66:A:MET:HE3  | 1:55:A:TYR:HE2  | 36                  | 0.14     | 0.02                | 0.14       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H    | 36                  | 0.14     | 0.01                | 0.14       |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H    | 36                  | 0.14     | 0.01                | 0.14       |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H    | 36                  | 0.14     | 0.01                | 0.14       |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H    | 36                  | 0.14     | 0.01                | 0.14       |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H    | 36                  | 0.14     | 0.01                | 0.14       |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H    | 36                  | 0.14     | 0.01                | 0.14       |
| (1,987)  | 1:12:A:PHE:H    | 1:11:A:GLN:HB2  | 36                  | 0.13     | 0.02                | 0.14       |
| (3,988)  | 1:12:A:PHE:H    | 1:11:A:GLN:HB2  | 36                  | 0.13     | 0.02                | 0.14       |
| (1,2424) | 1:39:A:ILE:HB   | 1:39:A:ILE:HD11 | 36                  | 0.11     | 0.0                 | 0.11       |
| (1,2424) | 1:39:A:ILE:HB   | 1:39:A:ILE:HD12 | 36                  | 0.11     | 0.0                 | 0.11       |
| (1,2424) | 1:39:A:ILE:HB   | 1:39:A:ILE:HD13 | 36                  | 0.11     | 0.0                 | 0.11       |
| (3,2427) | 1:39:A:ILE:HB   | 1:39:A:ILE:HD11 | 36                  | 0.11     | 0.0                 | 0.11       |
| (3,2427) | 1:39:A:ILE:HB   | 1:39:A:ILE:HD12 | 36                  | 0.11     | 0.0                 | 0.11       |
| (3,2427) | 1:39:A:ILE:HB   | 1:39:A:ILE:HD13 | 36                  | 0.11     | 0.0                 | 0.11       |
| (1,2322) | 1:80:A:SER:HB2  | 1:81:A:VAL:H    | 35                  | 0.22     | 0.02                | 0.22       |
| (3,2325) | 1:80:A:SER:HB2  | 1:81:A:VAL:H    | 35                  | 0.22     | 0.02                | 0.22       |
| (1,3116) | 1:55:A:TYR:HE1  | 1:68:A:ILE:HG21 | 35                  | 0.14     | 0.02                | 0.15       |
| (1,3116) | 1:55:A:TYR:HE1  | 1:68:A:ILE:HG22 | 35                  | 0.14     | 0.02                | 0.15       |
| (1,3116) | 1:55:A:TYR:HE1  | 1:68:A:ILE:HG23 | 35                  | 0.14     | 0.02                | 0.15       |
| (1,3116) | 1:55:A:TYR:HE2  | 1:68:A:ILE:HG21 | 35                  | 0.14     | 0.02                | 0.15       |
| (1,3116) | 1:55:A:TYR:HE2  | 1:68:A:ILE:HG22 | 35                  | 0.14     | 0.02                | 0.15       |
| (1,3116) | 1:55:A:TYR:HE2  | 1:68:A:ILE:HG23 | 35                  | 0.14     | 0.02                | 0.15       |
| (3,3122) | 1:55:A:TYR:HE1  | 1:68:A:ILE:HG21 | 35                  | 0.14     | 0.02                | 0.15       |
| (3,3122) | 1:55:A:TYR:HE1  | 1:68:A:ILE:HG22 | 35                  | 0.14     | 0.02                | 0.15       |
| (3,3122) | 1:55:A:TYR:HE1  | 1:68:A:ILE:HG23 | 35                  | 0.14     | 0.02                | 0.15       |
| (3,3122) | 1:55:A:TYR:HE2  | 1:68:A:ILE:HG21 | 35                  | 0.14     | 0.02                | 0.15       |
| (3,3122) | 1:55:A:TYR:HE2  | 1:68:A:ILE:HG22 | 35                  | 0.14     | 0.02                | 0.15       |
| (3,3122) | 1:55:A:TYR:HE2  | 1:68:A:ILE:HG23 | 35                  | 0.14     | 0.02                | 0.15       |
| (1,3100) | 1:79:A:TYR:HE1  | 1:55:A:TYR:HD1  | 35                  | 0.14     | 0.02                | 0.13       |
| (1,3100) | 1:79:A:TYR:HE1  | 1:55:A:TYR:HD2  | 35                  | 0.14     | 0.02                | 0.13       |
| (1,3100) | 1:79:A:TYR:HE2  | 1:55:A:TYR:HD1  | 35                  | 0.14     | 0.02                | 0.13       |
| (1,3100) | 1:79:A:TYR:HE2  | 1:55:A:TYR:HD2  | 35                  | 0.14     | 0.02                | 0.13       |
| (3,3106) | 1:79:A:TYR:HE1  | 1:55:A:TYR:HD1  | 35                  | 0.14     | 0.02                | 0.13       |
| (3,3106) | 1:79:A:TYR:HE1  | 1:55:A:TYR:HD2  | 35                  | 0.14     | 0.02                | 0.13       |
| (3,3106) | 1:79:A:TYR:HE2  | 1:55:A:TYR:HD1  | 35                  | 0.14     | 0.02                | 0.13       |
| (3,3106) | 1:79:A:TYR:HE2  | 1:55:A:TYR:HD2  | 35                  | 0.14     | 0.02                | 0.13       |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H    | 35                  | 0.12     | 0.01                | 0.12       |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H    | 35                  | 0.12     | 0.01                | 0.12       |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H    | 35                  | 0.12     | 0.01                | 0.12       |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H    | 35                  | 0.12     | 0.01                | 0.12       |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H    | 35                  | 0.12     | 0.01                | 0.12       |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H    | 35                  | 0.12     | 0.01                | 0.12       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H    | 35                  | 0.12     | 0.02                | 0.11       |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H    | 35                  | 0.12     | 0.02                | 0.11       |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H    | 35                  | 0.12     | 0.02                | 0.11       |
| (1,2699) | 1:23:A:GLU:HA   | 1:24:A:HIS:HA   | 35                  | 0.12     | 0.01                | 0.12       |
| (3,2703) | 1:23:A:GLU:HA   | 1:24:A:HIS:HA   | 35                  | 0.12     | 0.01                | 0.12       |
| (1,685)  | 1:23:A:GLU:H    | 1:23:A:GLU:HG3  | 34                  | 0.25     | 0.01                | 0.24       |
| (3,685)  | 1:23:A:GLU:H    | 1:23:A:GLU:HG3  | 34                  | 0.25     | 0.01                | 0.24       |
| (1,100)  | 1:22:A:SER:H    | 1:21:A:VAL:HB   | 34                  | 0.18     | 0.01                | 0.18       |
| (3,102)  | 1:22:A:SER:H    | 1:21:A:VAL:HB   | 34                  | 0.18     | 0.01                | 0.18       |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 34                  | 0.16     | 0.01                | 0.17       |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 34                  | 0.16     | 0.01                | 0.17       |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 34                  | 0.16     | 0.01                | 0.17       |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 34                  | 0.16     | 0.01                | 0.17       |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 34                  | 0.16     | 0.01                | 0.17       |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 34                  | 0.16     | 0.01                | 0.17       |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 34                  | 0.16     | 0.02                | 0.16       |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 34                  | 0.16     | 0.02                | 0.16       |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 34                  | 0.16     | 0.02                | 0.16       |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 34                  | 0.16     | 0.02                | 0.16       |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 34                  | 0.16     | 0.02                | 0.16       |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 34                  | 0.16     | 0.02                | 0.16       |
| (1,549)  | 1:71:A:VAL:H    | 1:70:A:ASN:HB2  | 34                  | 0.16     | 0.04                | 0.13       |
| (3,549)  | 1:71:A:VAL:H    | 1:70:A:ASN:HB2  | 34                  | 0.16     | 0.04                | 0.13       |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG21 | 34                  | 0.12     | 0.02                | 0.12       |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG22 | 34                  | 0.12     | 0.02                | 0.12       |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG23 | 34                  | 0.12     | 0.02                | 0.12       |
| (3,3020) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG21 | 34                  | 0.12     | 0.02                | 0.12       |
| (3,3020) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG22 | 34                  | 0.12     | 0.02                | 0.12       |
| (3,3020) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG23 | 34                  | 0.12     | 0.02                | 0.12       |
| (1,547)  | 1:71:A:VAL:H    | 1:71:A:VAL:HA   | 34                  | 0.12     | 0.0                 | 0.12       |
| (3,547)  | 1:71:A:VAL:H    | 1:71:A:VAL:HA   | 34                  | 0.12     | 0.0                 | 0.12       |
| (1,2431) | 1:82:A:ILE:HB   | 1:41:A:THR:H    | 33                  | 0.16     | 0.04                | 0.15       |
| (3,2434) | 1:82:A:ILE:HB   | 1:41:A:THR:H    | 33                  | 0.16     | 0.04                | 0.15       |
| (1,941)  | 1:34:A:SER:H    | 1:12:A:PHE:HA   | 33                  | 0.14     | 0.03                | 0.13       |
| (3,942)  | 1:34:A:SER:H    | 1:12:A:PHE:HA   | 33                  | 0.14     | 0.03                | 0.13       |
| (1,1020) | 1:48:A:GLU:H    | 1:48:A:GLU:HG3  | 33                  | 0.13     | 0.02                | 0.13       |
| (3,1019) | 1:48:A:GLU:H    | 1:48:A:GLU:HG3  | 33                  | 0.13     | 0.02                | 0.13       |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 33                  | 0.13     | 0.02                | 0.12       |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 33                  | 0.13     | 0.02                | 0.12       |
| (1,230)  | 1:13:A:THR:H    | 1:12:A:PHE:HD1  | 33                  | 0.12     | 0.02                | 0.12       |
| (1,230)  | 1:13:A:THR:H    | 1:12:A:PHE:HD2  | 33                  | 0.12     | 0.02                | 0.12       |
| (3,230)  | 1:13:A:THR:H    | 1:12:A:PHE:HD1  | 33                  | 0.12     | 0.02                | 0.12       |

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| Key      | Atom-1           | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|----------------|---------------------|----------|---------------------|------------|
| (3,230)  | 1:13:A:THR:H     | 1:12:A:PHE:HD2 | 33                  | 0.12     | 0.02                | 0.12       |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA | 32                  | 0.19     | 0.0                 | 0.19       |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA | 32                  | 0.19     | 0.0                 | 0.19       |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA | 32                  | 0.19     | 0.0                 | 0.19       |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA | 32                  | 0.19     | 0.0                 | 0.19       |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA | 32                  | 0.19     | 0.0                 | 0.19       |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA | 32                  | 0.19     | 0.0                 | 0.19       |
| (1,3134) | 1:65:A:TYR:HE1   | 1:30:A:GLU:HB2 | 32                  | 0.15     | 0.03                | 0.15       |
| (1,3134) | 1:65:A:TYR:HE2   | 1:30:A:GLU:HB2 | 32                  | 0.15     | 0.03                | 0.15       |
| (3,3140) | 1:65:A:TYR:HE1   | 1:30:A:GLU:HB2 | 32                  | 0.15     | 0.03                | 0.15       |
| (3,3140) | 1:65:A:TYR:HE2   | 1:30:A:GLU:HB2 | 32                  | 0.15     | 0.03                | 0.15       |
| (1,2021) | 1:50:A:THR:HG21  | 1:48:A:GLU:HG3 | 32                  | 0.13     | 0.02                | 0.12       |
| (1,2021) | 1:50:A:THR:HG22  | 1:48:A:GLU:HG3 | 32                  | 0.13     | 0.02                | 0.12       |
| (1,2021) | 1:50:A:THR:HG23  | 1:48:A:GLU:HG3 | 32                  | 0.13     | 0.02                | 0.12       |
| (3,2026) | 1:50:A:THR:HG21  | 1:48:A:GLU:HG3 | 32                  | 0.13     | 0.02                | 0.12       |
| (3,2026) | 1:50:A:THR:HG22  | 1:48:A:GLU:HG3 | 32                  | 0.13     | 0.02                | 0.12       |
| (3,2026) | 1:50:A:THR:HG23  | 1:48:A:GLU:HG3 | 32                  | 0.13     | 0.02                | 0.12       |
| (1,726)  | 1:49:A:LEU:H     | 1:48:A:GLU:HG3 | 32                  | 0.13     | 0.02                | 0.12       |
| (3,726)  | 1:49:A:LEU:H     | 1:48:A:GLU:HG3 | 32                  | 0.13     | 0.02                | 0.12       |
| (1,2996) | 1:15:A:ARG:HG2   | 1:93:A:SER:HB3 | 31                  | 0.16     | 0.03                | 0.16       |
| (3,3004) | 1:15:A:ARG:HG2   | 1:93:A:SER:HB3 | 31                  | 0.16     | 0.03                | 0.16       |
| (1,1379) | 1:83:A:ALA:HB1   | 1:91:A:ALA:HB1 | 31                  | 0.13     | 0.02                | 0.12       |
| (1,1379) | 1:83:A:ALA:HB1   | 1:91:A:ALA:HB2 | 31                  | 0.13     | 0.02                | 0.12       |
| (1,1379) | 1:83:A:ALA:HB1   | 1:91:A:ALA:HB3 | 31                  | 0.13     | 0.02                | 0.12       |
| (1,1379) | 1:83:A:ALA:HB2   | 1:91:A:ALA:HB1 | 31                  | 0.13     | 0.02                | 0.12       |
| (1,1379) | 1:83:A:ALA:HB2   | 1:91:A:ALA:HB2 | 31                  | 0.13     | 0.02                | 0.12       |
| (1,1379) | 1:83:A:ALA:HB2   | 1:91:A:ALA:HB3 | 31                  | 0.13     | 0.02                | 0.12       |
| (1,1379) | 1:83:A:ALA:HB3   | 1:91:A:ALA:HB1 | 31                  | 0.13     | 0.02                | 0.12       |
| (1,1379) | 1:83:A:ALA:HB3   | 1:91:A:ALA:HB2 | 31                  | 0.13     | 0.02                | 0.12       |
| (1,1379) | 1:83:A:ALA:HB3   | 1:91:A:ALA:HB3 | 31                  | 0.13     | 0.02                | 0.12       |
| (1,1384) | 1:91:A:ALA:HB1   | 1:83:A:ALA:HB1 | 31                  | 0.13     | 0.02                | 0.12       |
| (1,1384) | 1:91:A:ALA:HB1   | 1:83:A:ALA:HB2 | 31                  | 0.13     | 0.02                | 0.12       |
| (1,1384) | 1:91:A:ALA:HB1   | 1:83:A:ALA:HB3 | 31                  | 0.13     | 0.02                | 0.12       |
| (1,1384) | 1:91:A:ALA:HB2   | 1:83:A:ALA:HB1 | 31                  | 0.13     | 0.02                | 0.12       |
| (1,1384) | 1:91:A:ALA:HB2   | 1:83:A:ALA:HB2 | 31                  | 0.13     | 0.02                | 0.12       |
| (1,1384) | 1:91:A:ALA:HB2   | 1:83:A:ALA:HB3 | 31                  | 0.13     | 0.02                | 0.12       |
| (1,1384) | 1:91:A:ALA:HB3   | 1:83:A:ALA:HB1 | 31                  | 0.13     | 0.02                | 0.12       |
| (1,1384) | 1:91:A:ALA:HB3   | 1:83:A:ALA:HB2 | 31                  | 0.13     | 0.02                | 0.12       |
| (1,1384) | 1:91:A:ALA:HB3   | 1:83:A:ALA:HB3 | 31                  | 0.13     | 0.02                | 0.12       |
| (3,1383) | 1:83:A:ALA:HB1   | 1:91:A:ALA:HB1 | 31                  | 0.13     | 0.02                | 0.12       |
| (3,1383) | 1:83:A:ALA:HB1   | 1:91:A:ALA:HB2 | 31                  | 0.13     | 0.02                | 0.12       |
| (3,1383) | 1:83:A:ALA:HB1   | 1:91:A:ALA:HB3 | 31                  | 0.13     | 0.02                | 0.12       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB1  | 31                  | 0.13     | 0.02                | 0.12       |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB2  | 31                  | 0.13     | 0.02                | 0.12       |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB3  | 31                  | 0.13     | 0.02                | 0.12       |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB1  | 31                  | 0.13     | 0.02                | 0.12       |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB2  | 31                  | 0.13     | 0.02                | 0.12       |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB3  | 31                  | 0.13     | 0.02                | 0.12       |
| (3,1388) | 1:91:A:ALA:HB1  | 1:83:A:ALA:HB1  | 31                  | 0.13     | 0.02                | 0.12       |
| (3,1388) | 1:91:A:ALA:HB1  | 1:83:A:ALA:HB2  | 31                  | 0.13     | 0.02                | 0.12       |
| (3,1388) | 1:91:A:ALA:HB1  | 1:83:A:ALA:HB3  | 31                  | 0.13     | 0.02                | 0.12       |
| (3,1388) | 1:91:A:ALA:HB2  | 1:83:A:ALA:HB1  | 31                  | 0.13     | 0.02                | 0.12       |
| (3,1388) | 1:91:A:ALA:HB2  | 1:83:A:ALA:HB2  | 31                  | 0.13     | 0.02                | 0.12       |
| (3,1388) | 1:91:A:ALA:HB2  | 1:83:A:ALA:HB3  | 31                  | 0.13     | 0.02                | 0.12       |
| (3,1388) | 1:91:A:ALA:HB3  | 1:83:A:ALA:HB1  | 31                  | 0.13     | 0.02                | 0.12       |
| (3,1388) | 1:91:A:ALA:HB3  | 1:83:A:ALA:HB2  | 31                  | 0.13     | 0.02                | 0.12       |
| (3,1388) | 1:91:A:ALA:HB3  | 1:83:A:ALA:HB3  | 31                  | 0.13     | 0.02                | 0.12       |
| (1,933)  | 1:98:A:LYS:H    | 1:20:A:VAL:HG11 | 31                  | 0.13     | 0.02                | 0.12       |
| (1,933)  | 1:98:A:LYS:H    | 1:20:A:VAL:HG12 | 31                  | 0.13     | 0.02                | 0.12       |
| (1,933)  | 1:98:A:LYS:H    | 1:20:A:VAL:HG13 | 31                  | 0.13     | 0.02                | 0.12       |
| (3,934)  | 1:98:A:LYS:H    | 1:20:A:VAL:HG11 | 31                  | 0.13     | 0.02                | 0.12       |
| (3,934)  | 1:98:A:LYS:H    | 1:20:A:VAL:HG12 | 31                  | 0.13     | 0.02                | 0.12       |
| (3,934)  | 1:98:A:LYS:H    | 1:20:A:VAL:HG13 | 31                  | 0.13     | 0.02                | 0.12       |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 31                  | 0.12     | 0.01                | 0.12       |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 31                  | 0.12     | 0.01                | 0.12       |
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 31                  | 0.12     | 0.01                | 0.12       |
| (3,1712) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 31                  | 0.12     | 0.01                | 0.12       |
| (3,1712) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 31                  | 0.12     | 0.01                | 0.12       |
| (3,1712) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 31                  | 0.12     | 0.01                | 0.12       |
| (1,1387) | 1:91:A:ALA:HB1  | 1:12:A:PHE:HZ   | 30                  | 0.15     | 0.03                | 0.14       |
| (1,1387) | 1:91:A:ALA:HB2  | 1:12:A:PHE:HZ   | 30                  | 0.15     | 0.03                | 0.14       |
| (1,1387) | 1:91:A:ALA:HB3  | 1:12:A:PHE:HZ   | 30                  | 0.15     | 0.03                | 0.14       |
| (3,1391) | 1:91:A:ALA:HB1  | 1:12:A:PHE:HZ   | 30                  | 0.15     | 0.03                | 0.14       |
| (3,1391) | 1:91:A:ALA:HB2  | 1:12:A:PHE:HZ   | 30                  | 0.15     | 0.03                | 0.14       |
| (3,1391) | 1:91:A:ALA:HB3  | 1:12:A:PHE:HZ   | 30                  | 0.15     | 0.03                | 0.14       |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 30                  | 0.14     | 0.03                | 0.14       |
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 30                  | 0.14     | 0.03                | 0.14       |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 30                  | 0.14     | 0.03                | 0.14       |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 30                  | 0.14     | 0.03                | 0.14       |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 30                  | 0.14     | 0.03                | 0.14       |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 30                  | 0.14     | 0.03                | 0.14       |
| (1,2931) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 30                  | 0.14     | 0.03                | 0.13       |
| (3,2938) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 30                  | 0.14     | 0.03                | 0.13       |
| (1,3082) | 1:97:A:LEU:HB3  | 1:29:A:PHE:HE1  | 30                  | 0.14     | 0.02                | 0.14       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3082) | 1:97:A:LEU:HB3  | 1:29:A:PHE:HE2  | 30                  | 0.14     | 0.02                | 0.14       |
| (3,3088) | 1:97:A:LEU:HB3  | 1:29:A:PHE:HE1  | 30                  | 0.14     | 0.02                | 0.14       |
| (3,3088) | 1:97:A:LEU:HB3  | 1:29:A:PHE:HE2  | 30                  | 0.14     | 0.02                | 0.14       |
| (1,666)  | 1:72:A:THR:H    | 1:72:A:THR:HB   | 30                  | 0.11     | 0.01                | 0.11       |
| (3,666)  | 1:72:A:THR:H    | 1:72:A:THR:HB   | 30                  | 0.11     | 0.01                | 0.11       |
| (1,423)  | 1:69:A:HIS:H    | 1:69:A:HIS:HD2  | 29                  | 0.23     | 0.02                | 0.22       |
| (3,423)  | 1:69:A:HIS:H    | 1:69:A:HIS:HD2  | 29                  | 0.23     | 0.02                | 0.22       |
| (1,2403) | 1:66:A:MET:HE1  | 1:42:A:TRP:H    | 29                  | 0.15     | 0.02                | 0.15       |
| (1,2403) | 1:66:A:MET:HE2  | 1:42:A:TRP:H    | 29                  | 0.15     | 0.02                | 0.15       |
| (1,2403) | 1:66:A:MET:HE3  | 1:42:A:TRP:H    | 29                  | 0.15     | 0.02                | 0.15       |
| (3,2406) | 1:66:A:MET:HE1  | 1:42:A:TRP:H    | 29                  | 0.15     | 0.02                | 0.15       |
| (3,2406) | 1:66:A:MET:HE2  | 1:42:A:TRP:H    | 29                  | 0.15     | 0.02                | 0.15       |
| (3,2406) | 1:66:A:MET:HE3  | 1:42:A:TRP:H    | 29                  | 0.15     | 0.02                | 0.15       |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA   | 29                  | 0.14     | 0.02                | 0.14       |
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA   | 29                  | 0.14     | 0.02                | 0.14       |
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA   | 29                  | 0.14     | 0.02                | 0.14       |
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA   | 29                  | 0.14     | 0.02                | 0.14       |
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA   | 29                  | 0.14     | 0.02                | 0.14       |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA   | 29                  | 0.14     | 0.02                | 0.14       |
| (1,899)  | 1:44:A:LYS:H    | 1:43:A:TYR:HB2  | 29                  | 0.12     | 0.01                | 0.11       |
| (3,900)  | 1:44:A:LYS:H    | 1:43:A:TYR:HB2  | 29                  | 0.12     | 0.01                | 0.11       |
| (1,2802) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HB2  | 28                  | 0.18     | 0.04                | 0.19       |
| (3,2809) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HB2  | 28                  | 0.18     | 0.04                | 0.19       |
| (1,888)  | 1:80:A:SER:H    | 1:43:A:TYR:HB3  | 28                  | 0.16     | 0.03                | 0.16       |
| (3,889)  | 1:80:A:SER:H    | 1:43:A:TYR:HB3  | 28                  | 0.16     | 0.03                | 0.16       |
| (1,2937) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD1  | 28                  | 0.13     | 0.02                | 0.13       |
| (1,2937) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD2  | 28                  | 0.13     | 0.02                | 0.13       |
| (1,3137) | 1:65:A:TYR:HD1  | 1:30:A:GLU:HB3  | 28                  | 0.13     | 0.02                | 0.13       |
| (1,3137) | 1:65:A:TYR:HD2  | 1:30:A:GLU:HB3  | 28                  | 0.13     | 0.02                | 0.13       |
| (3,2944) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD1  | 28                  | 0.13     | 0.02                | 0.13       |
| (3,2944) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD2  | 28                  | 0.13     | 0.02                | 0.13       |
| (3,3143) | 1:65:A:TYR:HD1  | 1:30:A:GLU:HB3  | 28                  | 0.13     | 0.02                | 0.13       |
| (3,3143) | 1:65:A:TYR:HD2  | 1:30:A:GLU:HB3  | 28                  | 0.13     | 0.02                | 0.13       |
| (1,1990) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 28                  | 0.13     | 0.02                | 0.13       |
| (1,1990) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 28                  | 0.13     | 0.02                | 0.13       |
| (1,1990) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 28                  | 0.13     | 0.02                | 0.13       |
| (3,1993) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 28                  | 0.13     | 0.02                | 0.13       |
| (3,1993) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 28                  | 0.13     | 0.02                | 0.13       |
| (3,1993) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 28                  | 0.13     | 0.02                | 0.13       |
| (1,1508) | 1:66:A:MET:HE1  | 1:42:A:TRP:HZ3  | 27                  | 0.15     | 0.02                | 0.15       |
| (1,1508) | 1:66:A:MET:HE2  | 1:42:A:TRP:HZ3  | 27                  | 0.15     | 0.02                | 0.15       |
| (1,1508) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3  | 27                  | 0.15     | 0.02                | 0.15       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (3,1512) | 1:66:A:MET:HE1  | 1:42:A:TRP:HZ3  | 27                  | 0.15     | 0.02                | 0.15       |
| (3,1512) | 1:66:A:MET:HE2  | 1:42:A:TRP:HZ3  | 27                  | 0.15     | 0.02                | 0.15       |
| (3,1512) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3  | 27                  | 0.15     | 0.02                | 0.15       |
| (1,369)  | 1:18:A:ASN:H    | 1:17:A:GLN:HB2  | 27                  | 0.13     | 0.05                | 0.12       |
| (1,2649) | 1:17:A:GLN:HB2  | 1:18:A:ASN:H    | 27                  | 0.13     | 0.05                | 0.12       |
| (3,369)  | 1:18:A:ASN:H    | 1:17:A:GLN:HB2  | 27                  | 0.13     | 0.05                | 0.12       |
| (3,2653) | 1:17:A:GLN:HB2  | 1:18:A:ASN:H    | 27                  | 0.13     | 0.05                | 0.12       |
| (3,22)   | 1:89:A:GLY:H    | 1:85:A:LEU:H    | 26                  | 0.78     | 0.31                | 0.91       |
| (1,3190) | 1:79:A:TYR:HD1  | 1:29:A:PHE:HE1  | 26                  | 0.14     | 0.03                | 0.15       |
| (1,3190) | 1:79:A:TYR:HD1  | 1:29:A:PHE:HE2  | 26                  | 0.14     | 0.03                | 0.15       |
| (1,3190) | 1:79:A:TYR:HD2  | 1:29:A:PHE:HE1  | 26                  | 0.14     | 0.03                | 0.15       |
| (1,3190) | 1:79:A:TYR:HD2  | 1:29:A:PHE:HE2  | 26                  | 0.14     | 0.03                | 0.15       |
| (3,3196) | 1:79:A:TYR:HD1  | 1:29:A:PHE:HE1  | 26                  | 0.14     | 0.03                | 0.15       |
| (3,3196) | 1:79:A:TYR:HD1  | 1:29:A:PHE:HE2  | 26                  | 0.14     | 0.03                | 0.15       |
| (3,3196) | 1:79:A:TYR:HD2  | 1:29:A:PHE:HE1  | 26                  | 0.14     | 0.03                | 0.15       |
| (3,3196) | 1:79:A:TYR:HD2  | 1:29:A:PHE:HE2  | 26                  | 0.14     | 0.03                | 0.15       |
| (1,2416) | 1:10:A:ILE:HB   | 1:9:A:PRO:HA    | 26                  | 0.12     | 0.02                | 0.12       |
| (3,2419) | 1:10:A:ILE:HB   | 1:9:A:PRO:HA    | 26                  | 0.12     | 0.02                | 0.12       |
| (1,1357) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 26                  | 0.1      | 0.0                 | 0.1        |
| (1,1357) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 26                  | 0.1      | 0.0                 | 0.1        |
| (1,1357) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 26                  | 0.1      | 0.0                 | 0.1        |
| (3,1361) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 26                  | 0.1      | 0.0                 | 0.1        |
| (3,1361) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 26                  | 0.1      | 0.0                 | 0.1        |
| (3,1361) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 26                  | 0.1      | 0.0                 | 0.1        |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1  | 25                  | 0.13     | 0.02                | 0.12       |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2  | 25                  | 0.13     | 0.02                | 0.12       |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1  | 25                  | 0.13     | 0.02                | 0.12       |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2  | 25                  | 0.13     | 0.02                | 0.12       |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1  | 25                  | 0.13     | 0.02                | 0.12       |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2  | 25                  | 0.13     | 0.02                | 0.12       |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1  | 25                  | 0.13     | 0.02                | 0.12       |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2  | 25                  | 0.13     | 0.02                | 0.12       |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1  | 25                  | 0.13     | 0.02                | 0.12       |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2  | 25                  | 0.13     | 0.02                | 0.12       |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1  | 25                  | 0.13     | 0.02                | 0.12       |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2  | 25                  | 0.13     | 0.02                | 0.12       |
| (1,1510) | 1:66:A:MET:HE1  | 1:42:A:TRP:HE1  | 25                  | 0.13     | 0.02                | 0.13       |
| (1,1510) | 1:66:A:MET:HE2  | 1:42:A:TRP:HE1  | 25                  | 0.13     | 0.02                | 0.13       |
| (1,1510) | 1:66:A:MET:HE3  | 1:42:A:TRP:HE1  | 25                  | 0.13     | 0.02                | 0.13       |
| (1,3176) | 1:42:A:TRP:HE1  | 1:66:A:MET:HE1  | 25                  | 0.13     | 0.02                | 0.13       |
| (1,3176) | 1:42:A:TRP:HE1  | 1:66:A:MET:HE2  | 25                  | 0.13     | 0.02                | 0.13       |
| (1,3176) | 1:42:A:TRP:HE1  | 1:66:A:MET:HE3  | 25                  | 0.13     | 0.02                | 0.13       |

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| Key      | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (3,1514) | 1:66:A:MET:HE1 | 1:42:A:TRP:HE1  | 25                  | 0.13     | 0.02                | 0.13       |
| (3,1514) | 1:66:A:MET:HE2 | 1:42:A:TRP:HE1  | 25                  | 0.13     | 0.02                | 0.13       |
| (3,1514) | 1:66:A:MET:HE3 | 1:42:A:TRP:HE1  | 25                  | 0.13     | 0.02                | 0.13       |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 25                  | 0.13     | 0.02                | 0.13       |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 25                  | 0.13     | 0.02                | 0.13       |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 25                  | 0.13     | 0.02                | 0.13       |
| (3,2749) | 1:86:A:GLU:HG2 | 1:87:A:PRO:HA   | 24                  | 1.94     | 0.68                | 2.17       |
| (3,32)   | 1:88:A:ARG:H   | 1:86:A:GLU:HG2  | 24                  | 1.85     | 0.79                | 2.36       |
| (1,2437) | 1:90:A:GLU:HA  | 1:90:A:GLU:HG3  | 24                  | 0.28     | 0.0                 | 0.28       |
| (1,2756) | 1:90:A:GLU:HG3 | 1:90:A:GLU:HA   | 24                  | 0.28     | 0.0                 | 0.28       |
| (3,2440) | 1:90:A:GLU:HA  | 1:90:A:GLU:HG3  | 24                  | 0.28     | 0.0                 | 0.28       |
| (3,2763) | 1:90:A:GLU:HG3 | 1:90:A:GLU:HA   | 24                  | 0.28     | 0.0                 | 0.28       |
| (1,199)  | 1:90:A:GLU:H   | 1:10:A:ILE:HG21 | 24                  | 0.17     | 0.06                | 0.16       |
| (1,199)  | 1:90:A:GLU:H   | 1:10:A:ILE:HG22 | 24                  | 0.17     | 0.06                | 0.16       |
| (1,199)  | 1:90:A:GLU:H   | 1:10:A:ILE:HG23 | 24                  | 0.17     | 0.06                | 0.16       |
| (1,2550) | 1:92:A:ARG:HA  | 1:83:A:ALA:H    | 24                  | 0.16     | 0.03                | 0.16       |
| (3,2554) | 1:92:A:ARG:HA  | 1:83:A:ALA:H    | 24                  | 0.16     | 0.03                | 0.16       |
| (1,2974) | 1:65:A:TYR:HA  | 1:42:A:TRP:HZ2  | 24                  | 0.12     | 0.02                | 0.12       |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 24                  | 0.12     | 0.02                | 0.12       |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 24                  | 0.12     | 0.02                | 0.12       |
| (3,2982) | 1:65:A:TYR:HA  | 1:42:A:TRP:HZ2  | 24                  | 0.12     | 0.02                | 0.12       |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 24                  | 0.12     | 0.02                | 0.12       |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 24                  | 0.12     | 0.02                | 0.12       |
| (3,2529) | 1:87:A:PRO:HB3 | 1:86:A:GLU:HA   | 23                  | 1.21     | 0.43                | 1.36       |
| (1,1717) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG11 | 23                  | 0.15     | 0.03                | 0.15       |
| (1,1717) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG12 | 23                  | 0.15     | 0.03                | 0.15       |
| (1,1717) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG13 | 23                  | 0.15     | 0.03                | 0.15       |
| (1,1717) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG11 | 23                  | 0.15     | 0.03                | 0.15       |
| (1,1717) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG12 | 23                  | 0.15     | 0.03                | 0.15       |
| (1,1717) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG13 | 23                  | 0.15     | 0.03                | 0.15       |
| (1,1717) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG11 | 23                  | 0.15     | 0.03                | 0.15       |
| (1,1717) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG12 | 23                  | 0.15     | 0.03                | 0.15       |
| (1,1717) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG13 | 23                  | 0.15     | 0.03                | 0.15       |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG11 | 23                  | 0.15     | 0.03                | 0.15       |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG12 | 23                  | 0.15     | 0.03                | 0.15       |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG13 | 23                  | 0.15     | 0.03                | 0.15       |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG11 | 23                  | 0.15     | 0.03                | 0.15       |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG12 | 23                  | 0.15     | 0.03                | 0.15       |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG13 | 23                  | 0.15     | 0.03                | 0.15       |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG11 | 23                  | 0.15     | 0.03                | 0.15       |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG12 | 23                  | 0.15     | 0.03                | 0.15       |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG13 | 23                  | 0.15     | 0.03                | 0.15       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,366)  | 1:18:A:ASN:H    | 1:18:A:ASN:HB3  | 22                  | 0.21     | 0.01                | 0.2        |
| (1,2236) | 1:18:A:ASN:HB3  | 1:18:A:ASN:H    | 22                  | 0.21     | 0.01                | 0.2        |
| (3,366)  | 1:18:A:ASN:H    | 1:18:A:ASN:HB3  | 22                  | 0.21     | 0.01                | 0.2        |
| (3,2239) | 1:18:A:ASN:HB3  | 1:18:A:ASN:H    | 22                  | 0.21     | 0.01                | 0.2        |
| (1,35)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2  | 22                  | 0.14     | 0.02                | 0.14       |
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG21 | 22                  | 0.12     | 0.01                | 0.12       |
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG22 | 22                  | 0.12     | 0.01                | 0.12       |
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG23 | 22                  | 0.12     | 0.01                | 0.12       |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG21 | 22                  | 0.12     | 0.01                | 0.12       |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG22 | 22                  | 0.12     | 0.01                | 0.12       |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG23 | 22                  | 0.12     | 0.01                | 0.12       |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG21 | 22                  | 0.12     | 0.01                | 0.12       |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG22 | 22                  | 0.12     | 0.01                | 0.12       |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG23 | 22                  | 0.12     | 0.01                | 0.12       |
| (3,998)  | 1:79:A:TYR:H    | 1:94:A:THR:HG21 | 22                  | 0.12     | 0.01                | 0.12       |
| (3,998)  | 1:79:A:TYR:H    | 1:94:A:THR:HG22 | 22                  | 0.12     | 0.01                | 0.12       |
| (3,998)  | 1:79:A:TYR:H    | 1:94:A:THR:HG23 | 22                  | 0.12     | 0.01                | 0.12       |
| (1,1494) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 22                  | 0.12     | 0.01                | 0.12       |
| (1,1494) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 22                  | 0.12     | 0.01                | 0.12       |
| (1,1494) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 22                  | 0.12     | 0.01                | 0.12       |
| (3,1498) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 22                  | 0.12     | 0.01                | 0.12       |
| (3,1498) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 22                  | 0.12     | 0.01                | 0.12       |
| (3,1498) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 22                  | 0.12     | 0.01                | 0.12       |
| (3,2748) | 1:86:A:GLU:HG3  | 1:87:A:PRO:HA   | 21                  | 1.66     | 0.95                | 2.23       |
| (1,3131) | 1:65:A:TYR:HE1  | 1:63:A:CYS:HB3  | 21                  | 0.14     | 0.03                | 0.14       |
| (1,3131) | 1:65:A:TYR:HE2  | 1:63:A:CYS:HB3  | 21                  | 0.14     | 0.03                | 0.14       |
| (3,3137) | 1:65:A:TYR:HE1  | 1:63:A:CYS:HB3  | 21                  | 0.14     | 0.03                | 0.14       |
| (3,3137) | 1:65:A:TYR:HE2  | 1:63:A:CYS:HB3  | 21                  | 0.14     | 0.03                | 0.14       |
| (1,661)  | 1:7:A:ALA:H     | 1:6:A:THR:HA    | 21                  | 0.13     | 0.02                | 0.13       |
| (3,661)  | 1:7:A:ALA:H     | 1:6:A:THR:HA    | 21                  | 0.13     | 0.02                | 0.13       |
| (1,1513) | 1:66:A:MET:HE1  | 1:29:A:PHE:H    | 21                  | 0.13     | 0.02                | 0.12       |
| (1,1513) | 1:66:A:MET:HE2  | 1:29:A:PHE:H    | 21                  | 0.13     | 0.02                | 0.12       |
| (1,1513) | 1:66:A:MET:HE3  | 1:29:A:PHE:H    | 21                  | 0.13     | 0.02                | 0.12       |
| (3,1517) | 1:66:A:MET:HE1  | 1:29:A:PHE:H    | 21                  | 0.13     | 0.02                | 0.12       |
| (3,1517) | 1:66:A:MET:HE2  | 1:29:A:PHE:H    | 21                  | 0.13     | 0.02                | 0.12       |
| (3,1517) | 1:66:A:MET:HE3  | 1:29:A:PHE:H    | 21                  | 0.13     | 0.02                | 0.12       |
| (1,2145) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 21                  | 0.13     | 0.01                | 0.12       |
| (3,2148) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 21                  | 0.13     | 0.01                | 0.12       |
| (1,889)  | 1:80:A:SER:H    | 1:79:A:TYR:HB2  | 21                  | 0.11     | 0.01                | 0.11       |
| (3,890)  | 1:80:A:SER:H    | 1:79:A:TYR:HB2  | 21                  | 0.11     | 0.01                | 0.11       |
| (3,34)   | 1:88:A:ARG:H    | 1:86:A:GLU:HA   | 20                  | 3.25     | 0.02                | 3.24       |
| (3,2753) | 1:86:A:GLU:HB2  | 1:87:A:PRO:HA   | 20                  | 1.3      | 0.11                | 1.25       |

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| Key      | Atom-1          | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (3,2753) | 1:86:A:GLU:HB3  | 1:87:A:PRO:HA  | 20                  | 1.3      | 0.11                | 1.25       |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB2 | 20                  | 1.22     | 0.22                | 1.14       |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB3 | 20                  | 1.22     | 0.22                | 1.14       |
| (3,1149) | 1:86:A:GLU:H    | 1:87:A:PRO:HA  | 20                  | 0.84     | 0.05                | 0.82       |
| (3,862)  | 1:86:A:GLU:H    | 1:85:A:LEU:H   | 20                  | 0.34     | 0.01                | 0.34       |
| (1,3048) | 1:60:A:ASP:HB2  | 1:63:A:CYS:HB2 | 20                  | 0.25     | 0.02                | 0.25       |
| (3,3056) | 1:60:A:ASP:HB2  | 1:63:A:CYS:HB2 | 20                  | 0.25     | 0.02                | 0.25       |
| (1,1935) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 20                  | 0.22     | 0.0                 | 0.22       |
| (3,1938) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 20                  | 0.22     | 0.0                 | 0.22       |
| (1,2534) | 1:73:A:PRO:HD3  | 1:73:A:PRO:HB3 | 20                  | 0.21     | 0.01                | 0.21       |
| (3,2538) | 1:73:A:PRO:HD3  | 1:73:A:PRO:HB3 | 20                  | 0.21     | 0.01                | 0.21       |
| (1,3069) | 1:87:A:PRO:HD2  | 1:86:A:GLU:HB2 | 20                  | 0.17     | 0.02                | 0.17       |
| (1,3069) | 1:87:A:PRO:HD2  | 1:86:A:GLU:HB3 | 20                  | 0.17     | 0.02                | 0.17       |
| (1,148)  | 1:45:A:GLY:H    | 1:46:A:PRO:HD2 | 20                  | 0.14     | 0.02                | 0.14       |
| (1,810)  | 1:25:A:GLN:H    | 1:71:A:VAL:HB  | 20                  | 0.13     | 0.02                | 0.12       |
| (3,810)  | 1:25:A:GLN:H    | 1:71:A:VAL:HB  | 20                  | 0.13     | 0.02                | 0.12       |
| (1,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HB3 | 20                  | 0.13     | 0.01                | 0.13       |
| (3,39)   | 1:88:A:ARG:H    | 1:88:A:ARG:HB3 | 20                  | 0.13     | 0.01                | 0.13       |
| (1,2841) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA  | 20                  | 0.11     | 0.01                | 0.11       |
| (3,2848) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA  | 20                  | 0.11     | 0.01                | 0.11       |
| (1,281)  | 1:29:A:PHE:H    | 1:29:A:PHE:HB3 | 20                  | 0.1      | 0.01                | 0.1        |
| (3,281)  | 1:29:A:PHE:H    | 1:29:A:PHE:HB3 | 20                  | 0.1      | 0.01                | 0.1        |
| (1,149)  | 1:45:A:GLY:H    | 1:46:A:PRO:HD3 | 19                  | 0.27     | 0.04                | 0.28       |
| (1,1624) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2 | 18                  | 0.19     | 0.05                | 0.21       |
| (1,1624) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2 | 18                  | 0.19     | 0.05                | 0.21       |
| (1,1624) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2 | 18                  | 0.19     | 0.05                | 0.21       |
| (3,1628) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2 | 18                  | 0.19     | 0.05                | 0.21       |
| (3,1628) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2 | 18                  | 0.19     | 0.05                | 0.21       |
| (3,1628) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2 | 18                  | 0.19     | 0.05                | 0.21       |
| (1,488)  | 1:19:A:ILE:H    | 1:18:A:ASN:HB3 | 18                  | 0.15     | 0.02                | 0.16       |
| (3,488)  | 1:19:A:ILE:H    | 1:18:A:ASN:HB3 | 18                  | 0.15     | 0.02                | 0.16       |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 18                  | 0.14     | 0.02                | 0.15       |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 18                  | 0.14     | 0.02                | 0.15       |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 18                  | 0.14     | 0.02                | 0.15       |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 18                  | 0.14     | 0.02                | 0.15       |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 18                  | 0.14     | 0.02                | 0.15       |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 18                  | 0.14     | 0.02                | 0.15       |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 18                  | 0.14     | 0.02                | 0.15       |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 18                  | 0.14     | 0.02                | 0.15       |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 18                  | 0.14     | 0.02                | 0.15       |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 18                  | 0.14     | 0.02                | 0.15       |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 18                  | 0.14     | 0.02                | 0.15       |

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| Key      | Atom-1          | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 18                  | 0.14     | 0.02                | 0.15       |
| (1,1239) | 1:13:A:THR:HG21 | 1:34:A:SER:H   | 18                  | 0.13     | 0.02                | 0.13       |
| (1,1239) | 1:13:A:THR:HG22 | 1:34:A:SER:H   | 18                  | 0.13     | 0.02                | 0.13       |
| (1,1239) | 1:13:A:THR:HG23 | 1:34:A:SER:H   | 18                  | 0.13     | 0.02                | 0.13       |
| (3,1243) | 1:13:A:THR:HG21 | 1:34:A:SER:H   | 18                  | 0.13     | 0.02                | 0.13       |
| (3,1243) | 1:13:A:THR:HG22 | 1:34:A:SER:H   | 18                  | 0.13     | 0.02                | 0.13       |
| (3,1243) | 1:13:A:THR:HG23 | 1:34:A:SER:H   | 18                  | 0.13     | 0.02                | 0.13       |
| (1,1507) | 1:66:A:MET:HE1  | 1:42:A:TRP:HB2 | 18                  | 0.12     | 0.01                | 0.11       |
| (1,1507) | 1:66:A:MET:HE2  | 1:42:A:TRP:HB2 | 18                  | 0.12     | 0.01                | 0.11       |
| (1,1507) | 1:66:A:MET:HE3  | 1:42:A:TRP:HB2 | 18                  | 0.12     | 0.01                | 0.11       |
| (3,1511) | 1:66:A:MET:HE1  | 1:42:A:TRP:HB2 | 18                  | 0.12     | 0.01                | 0.11       |
| (3,1511) | 1:66:A:MET:HE2  | 1:42:A:TRP:HB2 | 18                  | 0.12     | 0.01                | 0.11       |
| (3,1511) | 1:66:A:MET:HE3  | 1:42:A:TRP:HB2 | 18                  | 0.12     | 0.01                | 0.11       |
| (1,2646) | 1:9:A:PRO:HB2   | 1:9:A:PRO:HD3  | 18                  | 0.11     | 0.01                | 0.11       |
| (3,2650) | 1:9:A:PRO:HB2   | 1:9:A:PRO:HD3  | 18                  | 0.11     | 0.01                | 0.11       |
| (1,3011) | 1:30:A:GLU:HB2  | 1:14:A:LYS:HE2 | 17                  | 0.13     | 0.02                | 0.13       |
| (3,3019) | 1:30:A:GLU:HB2  | 1:14:A:LYS:HE2 | 17                  | 0.13     | 0.02                | 0.13       |
| (1,1176) | 1:47:A:THR:H    | 1:44:A:LYS:HB3 | 17                  | 0.13     | 0.03                | 0.12       |
| (3,1180) | 1:47:A:THR:H    | 1:44:A:LYS:HB3 | 17                  | 0.13     | 0.03                | 0.12       |
| (1,513)  | 1:67:A:THR:H    | 1:66:A:MET:HG3 | 16                  | 0.22     | 0.03                | 0.21       |
| (3,513)  | 1:67:A:THR:H    | 1:66:A:MET:HG3 | 16                  | 0.22     | 0.03                | 0.21       |
| (1,1904) | 1:66:A:MET:HE1  | 1:43:A:TYR:H   | 16                  | 0.21     | 0.02                | 0.22       |
| (1,1904) | 1:66:A:MET:HE2  | 1:43:A:TYR:H   | 16                  | 0.21     | 0.02                | 0.22       |
| (1,1904) | 1:66:A:MET:HE3  | 1:43:A:TYR:H   | 16                  | 0.21     | 0.02                | 0.22       |
| (3,1907) | 1:66:A:MET:HE1  | 1:43:A:TYR:H   | 16                  | 0.21     | 0.02                | 0.22       |
| (3,1907) | 1:66:A:MET:HE2  | 1:43:A:TYR:H   | 16                  | 0.21     | 0.02                | 0.22       |
| (3,1907) | 1:66:A:MET:HE3  | 1:43:A:TYR:H   | 16                  | 0.21     | 0.02                | 0.22       |
| (1,274)  | 1:66:A:MET:H    | 1:66:A:MET:HG3 | 16                  | 0.18     | 0.01                | 0.18       |
| (3,274)  | 1:66:A:MET:H    | 1:66:A:MET:HG3 | 16                  | 0.18     | 0.01                | 0.18       |
| (1,1500) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2 | 16                  | 0.15     | 0.01                | 0.15       |
| (1,1500) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2 | 16                  | 0.15     | 0.01                | 0.15       |
| (1,1500) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2 | 16                  | 0.15     | 0.01                | 0.15       |
| (3,1504) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2 | 16                  | 0.15     | 0.01                | 0.15       |
| (3,1504) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2 | 16                  | 0.15     | 0.01                | 0.15       |
| (3,1504) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2 | 16                  | 0.15     | 0.01                | 0.15       |
| (1,1503) | 1:66:A:MET:HE1  | 1:66:A:MET:HG2 | 16                  | 0.12     | 0.0                 | 0.12       |
| (1,1503) | 1:66:A:MET:HE2  | 1:66:A:MET:HG2 | 16                  | 0.12     | 0.0                 | 0.12       |
| (1,1503) | 1:66:A:MET:HE3  | 1:66:A:MET:HG2 | 16                  | 0.12     | 0.0                 | 0.12       |
| (1,1550) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA   | 16                  | 0.12     | 0.01                | 0.11       |
| (1,1550) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA   | 16                  | 0.12     | 0.01                | 0.11       |
| (1,1550) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA   | 16                  | 0.12     | 0.01                | 0.11       |
| (3,1507) | 1:66:A:MET:HE1  | 1:66:A:MET:HG2 | 16                  | 0.12     | 0.0                 | 0.12       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (3,1507) | 1:66:A:MET:HE2  | 1:66:A:MET:HG2  | 16                  | 0.12     | 0.0                 | 0.12       |
| (3,1507) | 1:66:A:MET:HE3  | 1:66:A:MET:HG2  | 16                  | 0.12     | 0.0                 | 0.12       |
| (3,1554) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA    | 16                  | 0.12     | 0.01                | 0.11       |
| (3,1554) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA    | 16                  | 0.12     | 0.01                | 0.11       |
| (3,1554) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA    | 16                  | 0.12     | 0.01                | 0.11       |
| (1,198)  | 1:90:A:GLU:H    | 1:90:A:GLU:HB2  | 15                  | 0.14     | 0.02                | 0.15       |
| (3,198)  | 1:90:A:GLU:H    | 1:90:A:GLU:HB2  | 15                  | 0.14     | 0.02                | 0.15       |
| (1,1236) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3  | 15                  | 0.13     | 0.02                | 0.13       |
| (1,1236) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3  | 15                  | 0.13     | 0.02                | 0.13       |
| (1,1236) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3  | 15                  | 0.13     | 0.02                | 0.13       |
| (3,1240) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3  | 15                  | 0.13     | 0.02                | 0.13       |
| (3,1240) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3  | 15                  | 0.13     | 0.02                | 0.13       |
| (3,1240) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3  | 15                  | 0.13     | 0.02                | 0.13       |
| (1,1213) | 1:66:A:MET:H    | 1:28:A:THR:HA   | 15                  | 0.13     | 0.02                | 0.11       |
| (3,1217) | 1:66:A:MET:H    | 1:28:A:THR:HA   | 15                  | 0.13     | 0.02                | 0.11       |
| (1,2663) | 1:25:A:GLN:HB2  | 1:21:A:VAL:HG21 | 15                  | 0.12     | 0.02                | 0.11       |
| (1,2663) | 1:25:A:GLN:HB2  | 1:21:A:VAL:HG22 | 15                  | 0.12     | 0.02                | 0.11       |
| (1,2663) | 1:25:A:GLN:HB2  | 1:21:A:VAL:HG23 | 15                  | 0.12     | 0.02                | 0.11       |
| (3,2667) | 1:25:A:GLN:HB2  | 1:21:A:VAL:HG21 | 15                  | 0.12     | 0.02                | 0.11       |
| (3,2667) | 1:25:A:GLN:HB2  | 1:21:A:VAL:HG22 | 15                  | 0.12     | 0.02                | 0.11       |
| (3,2667) | 1:25:A:GLN:HB2  | 1:21:A:VAL:HG23 | 15                  | 0.12     | 0.02                | 0.11       |
| (1,590)  | 1:3:A:ASP:H     | 1:2:A:ILE:HA    | 14                  | 0.22     | 0.01                | 0.21       |
| (3,590)  | 1:3:A:ASP:H     | 1:2:A:ILE:HA    | 14                  | 0.22     | 0.01                | 0.21       |
| (1,1861) | 1:7:A:ALA:HB1   | 1:88:A:ARG:HA   | 14                  | 0.13     | 0.02                | 0.13       |
| (1,1861) | 1:7:A:ALA:HB2   | 1:88:A:ARG:HA   | 14                  | 0.13     | 0.02                | 0.13       |
| (1,1861) | 1:7:A:ALA:HB3   | 1:88:A:ARG:HA   | 14                  | 0.13     | 0.02                | 0.13       |
| (3,1864) | 1:7:A:ALA:HB1   | 1:88:A:ARG:HA   | 14                  | 0.13     | 0.02                | 0.13       |
| (3,1864) | 1:7:A:ALA:HB2   | 1:88:A:ARG:HA   | 14                  | 0.13     | 0.02                | 0.13       |
| (3,1864) | 1:7:A:ALA:HB3   | 1:88:A:ARG:HA   | 14                  | 0.13     | 0.02                | 0.13       |
| (1,2537) | 1:73:A:PRO:HG3  | 1:73:A:PRO:HA   | 14                  | 0.13     | 0.02                | 0.13       |
| (3,2541) | 1:73:A:PRO:HG3  | 1:73:A:PRO:HA   | 14                  | 0.13     | 0.02                | 0.13       |
| (1,339)  | 1:14:A:LYS:H    | 1:12:A:PHE:HD1  | 14                  | 0.12     | 0.02                | 0.12       |
| (1,339)  | 1:14:A:LYS:H    | 1:12:A:PHE:HD2  | 14                  | 0.12     | 0.02                | 0.12       |
| (3,339)  | 1:14:A:LYS:H    | 1:12:A:PHE:HD1  | 14                  | 0.12     | 0.02                | 0.12       |
| (3,339)  | 1:14:A:LYS:H    | 1:12:A:PHE:HD2  | 14                  | 0.12     | 0.02                | 0.12       |
| (1,1896) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3  | 14                  | 0.12     | 0.01                | 0.12       |
| (1,1896) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3  | 14                  | 0.12     | 0.01                | 0.12       |
| (1,1896) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3  | 14                  | 0.12     | 0.01                | 0.12       |
| (3,1899) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3  | 14                  | 0.12     | 0.01                | 0.12       |
| (3,1899) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3  | 14                  | 0.12     | 0.01                | 0.12       |
| (3,1899) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3  | 14                  | 0.12     | 0.01                | 0.12       |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD11 | 13                  | 0.16     | 0.03                | 0.16       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD12 | 13                  | 0.16     | 0.03                | 0.16       |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD13 | 13                  | 0.16     | 0.03                | 0.16       |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD11 | 13                  | 0.16     | 0.03                | 0.16       |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD12 | 13                  | 0.16     | 0.03                | 0.16       |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD13 | 13                  | 0.16     | 0.03                | 0.16       |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD11 | 13                  | 0.16     | 0.03                | 0.16       |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD12 | 13                  | 0.16     | 0.03                | 0.16       |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD13 | 13                  | 0.16     | 0.03                | 0.16       |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD11 | 13                  | 0.16     | 0.03                | 0.16       |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD12 | 13                  | 0.16     | 0.03                | 0.16       |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD13 | 13                  | 0.16     | 0.03                | 0.16       |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD11 | 13                  | 0.16     | 0.03                | 0.16       |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD12 | 13                  | 0.16     | 0.03                | 0.16       |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD13 | 13                  | 0.16     | 0.03                | 0.16       |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD11 | 13                  | 0.16     | 0.03                | 0.16       |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD12 | 13                  | 0.16     | 0.03                | 0.16       |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD13 | 13                  | 0.16     | 0.03                | 0.16       |
| (1,2460) | 1:4:A:PRO:HD3   | 1:3:A:ASP:HA    | 13                  | 0.15     | 0.02                | 0.15       |
| (3,2463) | 1:4:A:PRO:HD3   | 1:3:A:ASP:HA    | 13                  | 0.15     | 0.02                | 0.15       |
| (1,2099) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HA   | 13                  | 0.14     | 0.03                | 0.13       |
| (1,2099) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HA   | 13                  | 0.14     | 0.03                | 0.13       |
| (1,2099) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HA   | 13                  | 0.14     | 0.03                | 0.13       |
| (3,2102) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HA   | 13                  | 0.14     | 0.03                | 0.13       |
| (3,2102) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HA   | 13                  | 0.14     | 0.03                | 0.13       |
| (3,2102) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HA   | 13                  | 0.14     | 0.03                | 0.13       |
| (1,55)   | 1:42:A:TRP:H    | 1:42:A:TRP:HB3  | 13                  | 0.1      | 0.0                 | 0.1        |
| (3,57)   | 1:42:A:TRP:H    | 1:42:A:TRP:HB3  | 13                  | 0.1      | 0.0                 | 0.1        |
| (1,2801) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HG2  | 12                  | 0.22     | 0.0                 | 0.22       |
| (3,2808) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HG2  | 12                  | 0.22     | 0.0                 | 0.22       |
| (1,3185) | 1:43:A:TYR:HD1  | 1:44:A:LYS:H    | 12                  | 0.12     | 0.01                | 0.12       |
| (1,3185) | 1:43:A:TYR:HD2  | 1:44:A:LYS:H    | 12                  | 0.12     | 0.01                | 0.12       |
| (3,3191) | 1:43:A:TYR:HD1  | 1:44:A:LYS:H    | 12                  | 0.12     | 0.01                | 0.12       |
| (3,3191) | 1:43:A:TYR:HD2  | 1:44:A:LYS:H    | 12                  | 0.12     | 0.01                | 0.12       |
| (1,2608) | 1:60:A:ASP:HB3  | 1:60:A:ASP:H    | 12                  | 0.11     | 0.01                | 0.11       |
| (1,2609) | 1:60:A:ASP:HB3  | 1:60:A:ASP:H    | 12                  | 0.11     | 0.01                | 0.11       |
| (3,2612) | 1:60:A:ASP:HB3  | 1:60:A:ASP:H    | 12                  | 0.11     | 0.01                | 0.11       |
| (3,2613) | 1:60:A:ASP:HB3  | 1:60:A:ASP:H    | 12                  | 0.11     | 0.01                | 0.11       |
| (1,165)  | 1:10:A:ILE:H    | 1:9:A:PRO:HB2   | 12                  | 0.11     | 0.01                | 0.11       |
| (3,165)  | 1:10:A:ILE:H    | 1:9:A:PRO:HB2   | 12                  | 0.11     | 0.01                | 0.11       |
| (1,2678) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HA   | 11                  | 0.29     | 0.0                 | 0.29       |
| (3,2682) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HA   | 11                  | 0.29     | 0.0                 | 0.29       |
| (1,2676) | 1:53:A:GLN:HA   | 1:53:A:GLN:HB2  | 11                  | 0.19     | 0.0                 | 0.19       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (3,2680) | 1:53:A:GLN:HA   | 1:53:A:GLN:HB2  | 11                  | 0.19     | 0.0                 | 0.19       |
| (1,1174) | 1:91:A:ALA:H    | 1:84:A:ARG:HA   | 11                  | 0.15     | 0.02                | 0.15       |
| (3,1178) | 1:91:A:ALA:H    | 1:84:A:ARG:HA   | 11                  | 0.15     | 0.02                | 0.15       |
| (1,3211) | 1:69:A:HIS:HE1  | 1:67:A:THR:HB   | 11                  | 0.14     | 0.03                | 0.14       |
| (3,3217) | 1:69:A:HIS:HE1  | 1:67:A:THR:HB   | 11                  | 0.14     | 0.03                | 0.14       |
| (1,1226) | 1:101:A:LEU:H   | 1:22:A:SER:HA   | 11                  | 0.14     | 0.03                | 0.14       |
| (3,1230) | 1:101:A:LEU:H   | 1:22:A:SER:HA   | 11                  | 0.14     | 0.03                | 0.14       |
| (1,3132) | 1:65:A:TYR:HE1  | 1:63:A:CYS:HB2  | 11                  | 0.14     | 0.02                | 0.13       |
| (1,3132) | 1:65:A:TYR:HE2  | 1:63:A:CYS:HB2  | 11                  | 0.14     | 0.02                | 0.13       |
| (3,3138) | 1:65:A:TYR:HE1  | 1:63:A:CYS:HB2  | 11                  | 0.14     | 0.02                | 0.13       |
| (3,3138) | 1:65:A:TYR:HE2  | 1:63:A:CYS:HB2  | 11                  | 0.14     | 0.02                | 0.13       |
| (1,3169) | 1:69:A:HIS:HD2  | 1:69:A:HIS:HB3  | 11                  | 0.13     | 0.01                | 0.13       |
| (3,3175) | 1:69:A:HIS:HD2  | 1:69:A:HIS:HB3  | 11                  | 0.13     | 0.01                | 0.13       |
| (1,3033) | 1:44:A:LYS:HE2  | 1:79:A:TYR:HE1  | 11                  | 0.13     | 0.02                | 0.12       |
| (1,3033) | 1:44:A:LYS:HE2  | 1:79:A:TYR:HE2  | 11                  | 0.13     | 0.02                | 0.12       |
| (3,3041) | 1:44:A:LYS:HE2  | 1:79:A:TYR:HE1  | 11                  | 0.13     | 0.02                | 0.12       |
| (3,3041) | 1:44:A:LYS:HE2  | 1:79:A:TYR:HE2  | 11                  | 0.13     | 0.02                | 0.12       |
| (1,1149) | 1:54:A:LYS:H    | 1:53:A:GLN:HG3  | 11                  | 0.12     | 0.03                | 0.11       |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD21 | 11                  | 0.12     | 0.01                | 0.12       |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD22 | 11                  | 0.12     | 0.01                | 0.12       |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD23 | 11                  | 0.12     | 0.01                | 0.12       |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD21 | 11                  | 0.12     | 0.01                | 0.12       |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD22 | 11                  | 0.12     | 0.01                | 0.12       |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD23 | 11                  | 0.12     | 0.01                | 0.12       |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD21 | 11                  | 0.12     | 0.01                | 0.12       |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD22 | 11                  | 0.12     | 0.01                | 0.12       |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD23 | 11                  | 0.12     | 0.01                | 0.12       |
| (3,1152) | 1:54:A:LYS:H    | 1:53:A:GLN:HG3  | 11                  | 0.12     | 0.03                | 0.11       |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD21 | 11                  | 0.12     | 0.01                | 0.12       |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD22 | 11                  | 0.12     | 0.01                | 0.12       |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD23 | 11                  | 0.12     | 0.01                | 0.12       |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD21 | 11                  | 0.12     | 0.01                | 0.12       |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD22 | 11                  | 0.12     | 0.01                | 0.12       |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD23 | 11                  | 0.12     | 0.01                | 0.12       |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD21 | 11                  | 0.12     | 0.01                | 0.12       |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD22 | 11                  | 0.12     | 0.01                | 0.12       |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD23 | 11                  | 0.12     | 0.01                | 0.12       |
| (1,3133) | 1:65:A:TYR:HE1  | 1:60:A:ASP:HB3  | 11                  | 0.12     | 0.01                | 0.12       |
| (1,3133) | 1:65:A:TYR:HE2  | 1:60:A:ASP:HB3  | 11                  | 0.12     | 0.01                | 0.12       |
| (3,3139) | 1:65:A:TYR:HE1  | 1:60:A:ASP:HB3  | 11                  | 0.12     | 0.01                | 0.12       |
| (3,3139) | 1:65:A:TYR:HE2  | 1:60:A:ASP:HB3  | 11                  | 0.12     | 0.01                | 0.12       |
| (1,1484) | 1:81:A:VAL:HB   | 1:42:A:TRP:HE1  | 11                  | 0.12     | 0.01                | 0.11       |

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| Key      | Atom-1          | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (3,1488) | 1:81:A:VAL:HB   | 1:42:A:TRP:HE1 | 11                  | 0.12     | 0.01                | 0.11       |
| (1,203)  | 1:90:A:GLU:H    | 1:91:A:ALA:H   | 11                  | 0.1      | 0.0                 | 0.1        |
| (3,203)  | 1:90:A:GLU:H    | 1:91:A:ALA:H   | 11                  | 0.1      | 0.0                 | 0.1        |
| (1,2479) | 1:9:A:PRO:HD2   | 1:8:A:GLU:HA   | 10                  | 0.14     | 0.04                | 0.13       |
| (3,2482) | 1:9:A:PRO:HD2   | 1:8:A:GLU:HA   | 10                  | 0.14     | 0.04                | 0.13       |
| (1,2014) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD1 | 10                  | 0.13     | 0.02                | 0.12       |
| (1,2014) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD2 | 10                  | 0.13     | 0.02                | 0.12       |
| (3,2019) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD1 | 10                  | 0.13     | 0.02                | 0.12       |
| (3,2019) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD2 | 10                  | 0.13     | 0.02                | 0.12       |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1 | 10                  | 0.13     | 0.01                | 0.12       |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2 | 10                  | 0.13     | 0.01                | 0.12       |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3 | 10                  | 0.13     | 0.01                | 0.12       |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1 | 10                  | 0.13     | 0.01                | 0.12       |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2 | 10                  | 0.13     | 0.01                | 0.12       |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3 | 10                  | 0.13     | 0.01                | 0.12       |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1 | 10                  | 0.13     | 0.01                | 0.12       |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2 | 10                  | 0.13     | 0.01                | 0.12       |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3 | 10                  | 0.13     | 0.01                | 0.12       |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1 | 10                  | 0.13     | 0.01                | 0.12       |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2 | 10                  | 0.13     | 0.01                | 0.12       |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3 | 10                  | 0.13     | 0.01                | 0.12       |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1 | 10                  | 0.13     | 0.01                | 0.12       |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2 | 10                  | 0.13     | 0.01                | 0.12       |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3 | 10                  | 0.13     | 0.01                | 0.12       |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1 | 10                  | 0.13     | 0.01                | 0.12       |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2 | 10                  | 0.13     | 0.01                | 0.12       |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3 | 10                  | 0.13     | 0.01                | 0.12       |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1 | 10                  | 0.13     | 0.01                | 0.12       |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2 | 10                  | 0.13     | 0.01                | 0.12       |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3 | 10                  | 0.13     | 0.01                | 0.12       |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1 | 10                  | 0.13     | 0.01                | 0.12       |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2 | 10                  | 0.13     | 0.01                | 0.12       |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3 | 10                  | 0.13     | 0.01                | 0.12       |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1 | 10                  | 0.13     | 0.01                | 0.12       |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2 | 10                  | 0.13     | 0.01                | 0.12       |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3 | 10                  | 0.13     | 0.01                | 0.12       |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1 | 10                  | 0.13     | 0.01                | 0.12       |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2 | 10                  | 0.13     | 0.01                | 0.12       |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3 | 10                  | 0.13     | 0.01                | 0.12       |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1 | 10                  | 0.13     | 0.01                | 0.12       |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2 | 10                  | 0.13     | 0.01                | 0.12       |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3 | 10                  | 0.13     | 0.01                | 0.12       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1  | 10                  | 0.13     | 0.01                | 0.12       |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2  | 10                  | 0.13     | 0.01                | 0.12       |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3  | 10                  | 0.13     | 0.01                | 0.12       |
| (1,3040) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG21 | 10                  | 0.12     | 0.02                | 0.12       |
| (1,3040) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG22 | 10                  | 0.12     | 0.02                | 0.12       |
| (1,3040) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG23 | 10                  | 0.12     | 0.02                | 0.12       |
| (3,3048) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG21 | 10                  | 0.12     | 0.02                | 0.12       |
| (3,3048) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG22 | 10                  | 0.12     | 0.02                | 0.12       |
| (3,3048) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG23 | 10                  | 0.12     | 0.02                | 0.12       |
| (1,709)  | 1:16:A:ILE:H    | 1:31:A:CYS:HB2  | 10                  | 0.11     | 0.01                | 0.11       |
| (3,709)  | 1:16:A:ILE:H    | 1:31:A:CYS:HB2  | 10                  | 0.11     | 0.01                | 0.11       |
| (1,3194) | 1:29:A:PHE:HZ   | 1:19:A:ILE:HG21 | 10                  | 0.11     | 0.01                | 0.11       |
| (1,3194) | 1:29:A:PHE:HZ   | 1:19:A:ILE:HG22 | 10                  | 0.11     | 0.01                | 0.11       |
| (1,3194) | 1:29:A:PHE:HZ   | 1:19:A:ILE:HG23 | 10                  | 0.11     | 0.01                | 0.11       |
| (3,3200) | 1:29:A:PHE:HZ   | 1:19:A:ILE:HG21 | 10                  | 0.11     | 0.01                | 0.11       |
| (3,3200) | 1:29:A:PHE:HZ   | 1:19:A:ILE:HG22 | 10                  | 0.11     | 0.01                | 0.11       |
| (3,3200) | 1:29:A:PHE:HZ   | 1:19:A:ILE:HG23 | 10                  | 0.11     | 0.01                | 0.11       |
| (1,742)  | 1:76:A:GLU:H    | 1:77:A:GLY:H    | 10                  | 0.11     | 0.0                 | 0.11       |
| (3,742)  | 1:76:A:GLU:H    | 1:77:A:GLY:H    | 10                  | 0.11     | 0.0                 | 0.11       |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD11 | 9                   | 0.12     | 0.02                | 0.12       |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD12 | 9                   | 0.12     | 0.02                | 0.12       |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD13 | 9                   | 0.12     | 0.02                | 0.12       |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD11 | 9                   | 0.12     | 0.02                | 0.12       |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD12 | 9                   | 0.12     | 0.02                | 0.12       |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD13 | 9                   | 0.12     | 0.02                | 0.12       |
| (1,3197) | 1:42:A:TRP:HZ2  | 1:30:A:GLU:HA   | 9                   | 0.12     | 0.01                | 0.12       |
| (3,3203) | 1:42:A:TRP:HZ2  | 1:30:A:GLU:HA   | 9                   | 0.12     | 0.01                | 0.12       |
| (1,863)  | 1:86:A:GLU:H    | 1:85:A:LEU:HB3  | 9                   | 0.12     | 0.01                | 0.12       |
| (3,863)  | 1:86:A:GLU:H    | 1:85:A:LEU:HB3  | 9                   | 0.12     | 0.01                | 0.12       |
| (1,609)  | 1:43:A:TYR:H    | 1:42:A:TRP:HB2  | 9                   | 0.11     | 0.01                | 0.11       |
| (1,1261) | 1:67:A:THR:HG21 | 1:56:A:ASN:H    | 9                   | 0.11     | 0.01                | 0.11       |
| (1,1261) | 1:67:A:THR:HG22 | 1:56:A:ASN:H    | 9                   | 0.11     | 0.01                | 0.11       |
| (1,1261) | 1:67:A:THR:HG23 | 1:56:A:ASN:H    | 9                   | 0.11     | 0.01                | 0.11       |
| (3,609)  | 1:43:A:TYR:H    | 1:42:A:TRP:HB2  | 9                   | 0.11     | 0.01                | 0.11       |
| (3,1265) | 1:67:A:THR:HG21 | 1:56:A:ASN:H    | 9                   | 0.11     | 0.01                | 0.11       |
| (3,1265) | 1:67:A:THR:HG22 | 1:56:A:ASN:H    | 9                   | 0.11     | 0.01                | 0.11       |
| (3,1265) | 1:67:A:THR:HG23 | 1:56:A:ASN:H    | 9                   | 0.11     | 0.01                | 0.11       |
| (1,2467) | 1:4:A:PRO:HB2   | 1:4:A:PRO:HD2   | 8                   | 0.25     | 0.02                | 0.25       |
| (3,2470) | 1:4:A:PRO:HB2   | 1:4:A:PRO:HD2   | 8                   | 0.25     | 0.02                | 0.25       |
| (1,1530) | 1:2:A:ILE:HG21  | 1:2:A:ILE:HA    | 8                   | 0.18     | 0.01                | 0.18       |
| (1,1530) | 1:2:A:ILE:HG22  | 1:2:A:ILE:HA    | 8                   | 0.18     | 0.01                | 0.18       |
| (1,1530) | 1:2:A:ILE:HG23  | 1:2:A:ILE:HA    | 8                   | 0.18     | 0.01                | 0.18       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (3,1534) | 1:2:A:ILE:HG21  | 1:2:A:ILE:HA    | 8                   | 0.18     | 0.01                | 0.18       |
| (3,1534) | 1:2:A:ILE:HG22  | 1:2:A:ILE:HA    | 8                   | 0.18     | 0.01                | 0.18       |
| (3,1534) | 1:2:A:ILE:HG23  | 1:2:A:ILE:HA    | 8                   | 0.18     | 0.01                | 0.18       |
| (1,1543) | 1:2:A:ILE:HG12  | 1:2:A:ILE:HA    | 8                   | 0.16     | 0.01                | 0.16       |
| (3,1547) | 1:2:A:ILE:HG12  | 1:2:A:ILE:HA    | 8                   | 0.16     | 0.01                | 0.16       |
| (1,1257) | 1:67:A:THR:HG21 | 1:26:A:SER:HB2  | 8                   | 0.15     | 0.02                | 0.16       |
| (1,1257) | 1:67:A:THR:HG22 | 1:26:A:SER:HB2  | 8                   | 0.15     | 0.02                | 0.16       |
| (1,1257) | 1:67:A:THR:HG23 | 1:26:A:SER:HB2  | 8                   | 0.15     | 0.02                | 0.16       |
| (3,1261) | 1:67:A:THR:HG21 | 1:26:A:SER:HB2  | 8                   | 0.15     | 0.02                | 0.16       |
| (3,1261) | 1:67:A:THR:HG22 | 1:26:A:SER:HB2  | 8                   | 0.15     | 0.02                | 0.16       |
| (3,1261) | 1:67:A:THR:HG23 | 1:26:A:SER:HB2  | 8                   | 0.15     | 0.02                | 0.16       |
| (1,1217) | 1:69:A:HIS:H    | 1:56:A:ASN:H    | 8                   | 0.12     | 0.02                | 0.12       |
| (3,1221) | 1:69:A:HIS:H    | 1:56:A:ASN:H    | 8                   | 0.12     | 0.02                | 0.12       |
| (1,2331) | 1:26:A:SER:HA   | 1:68:A:ILE:HG21 | 8                   | 0.12     | 0.01                | 0.12       |
| (1,2331) | 1:26:A:SER:HA   | 1:68:A:ILE:HG22 | 8                   | 0.12     | 0.01                | 0.12       |
| (1,2331) | 1:26:A:SER:HA   | 1:68:A:ILE:HG23 | 8                   | 0.12     | 0.01                | 0.12       |
| (3,2334) | 1:26:A:SER:HA   | 1:68:A:ILE:HG21 | 8                   | 0.12     | 0.01                | 0.12       |
| (3,2334) | 1:26:A:SER:HA   | 1:68:A:ILE:HG22 | 8                   | 0.12     | 0.01                | 0.12       |
| (3,2334) | 1:26:A:SER:HA   | 1:68:A:ILE:HG23 | 8                   | 0.12     | 0.01                | 0.12       |
| (1,419)  | 1:69:A:HIS:H    | 1:54:A:LYS:HA   | 8                   | 0.11     | 0.02                | 0.11       |
| (3,419)  | 1:69:A:HIS:H    | 1:54:A:LYS:HA   | 8                   | 0.11     | 0.02                | 0.11       |
| (1,1002) | 1:5:A:PHE:H     | 1:4:A:PRO:HA    | 7                   | 0.16     | 0.03                | 0.15       |
| (3,1003) | 1:5:A:PHE:H     | 1:4:A:PRO:HA    | 7                   | 0.16     | 0.03                | 0.15       |
| (1,2745) | 1:86:A:GLU:HG2  | 1:86:A:GLU:H    | 7                   | 0.13     | 0.03                | 0.13       |
| (1,2745) | 1:86:A:GLU:HG3  | 1:86:A:GLU:H    | 7                   | 0.13     | 0.03                | 0.13       |
| (1,3158) | 1:42:A:TRP:HD1  | 1:41:A:THR:HA   | 7                   | 0.13     | 0.02                | 0.12       |
| (3,3164) | 1:42:A:TRP:HD1  | 1:41:A:THR:HA   | 7                   | 0.13     | 0.02                | 0.12       |
| (1,111)  | 1:63:A:CYS:H    | 1:60:A:ASP:H    | 7                   | 0.12     | 0.02                | 0.12       |
| (3,113)  | 1:63:A:CYS:H    | 1:60:A:ASP:H    | 7                   | 0.12     | 0.02                | 0.12       |
| (1,365)  | 1:18:A:ASN:H    | 1:18:A:ASN:HB2  | 6                   | 0.24     | 0.01                | 0.24       |
| (3,365)  | 1:18:A:ASN:H    | 1:18:A:ASN:HB2  | 6                   | 0.24     | 0.01                | 0.24       |
| (1,2879) | 1:102:A:ARG:HD3 | 1:102:A:ARG:HG2 | 6                   | 0.21     | 0.0                 | 0.21       |
| (3,2886) | 1:102:A:ARG:HD3 | 1:102:A:ARG:HG2 | 6                   | 0.21     | 0.0                 | 0.21       |
| (1,919)  | 1:37:A:ASP:H    | 1:36:A:ASP:HB2  | 6                   | 0.2      | 0.03                | 0.21       |
| (1,2598) | 1:36:A:ASP:HB2  | 1:37:A:ASP:H    | 6                   | 0.2      | 0.03                | 0.21       |
| (3,920)  | 1:37:A:ASP:H    | 1:36:A:ASP:HB2  | 6                   | 0.2      | 0.03                | 0.21       |
| (3,2602) | 1:36:A:ASP:HB2  | 1:37:A:ASP:H    | 6                   | 0.2      | 0.03                | 0.21       |
| (1,684)  | 1:23:A:GLU:H    | 1:23:A:GLU:HB3  | 6                   | 0.17     | 0.0                 | 0.17       |
| (3,684)  | 1:23:A:GLU:H    | 1:23:A:GLU:HB3  | 6                   | 0.17     | 0.0                 | 0.17       |
| (1,2237) | 1:18:A:ASN:HB2  | 1:18:A:ASN:H    | 6                   | 0.14     | 0.01                | 0.14       |
| (3,2240) | 1:18:A:ASN:HB2  | 1:18:A:ASN:H    | 6                   | 0.14     | 0.01                | 0.14       |
| (1,2087) | 1:85:A:LEU:HD11 | 1:39:A:ILE:H    | 6                   | 0.14     | 0.03                | 0.13       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2087) | 1:85:A:LEU:HD12 | 1:39:A:ILE:H    | 6                   | 0.14     | 0.03                | 0.13       |
| (1,2087) | 1:85:A:LEU:HD13 | 1:39:A:ILE:H    | 6                   | 0.14     | 0.03                | 0.13       |
| (1,971)  | 1:21:A:VAL:H    | 1:21:A:VAL:HG21 | 6                   | 0.13     | 0.01                | 0.13       |
| (1,971)  | 1:21:A:VAL:H    | 1:21:A:VAL:HG22 | 6                   | 0.13     | 0.01                | 0.13       |
| (1,971)  | 1:21:A:VAL:H    | 1:21:A:VAL:HG23 | 6                   | 0.13     | 0.01                | 0.13       |
| (3,972)  | 1:21:A:VAL:H    | 1:21:A:VAL:HG21 | 6                   | 0.13     | 0.01                | 0.13       |
| (3,972)  | 1:21:A:VAL:H    | 1:21:A:VAL:HG22 | 6                   | 0.13     | 0.01                | 0.13       |
| (3,972)  | 1:21:A:VAL:H    | 1:21:A:VAL:HG23 | 6                   | 0.13     | 0.01                | 0.13       |
| (1,2942) | 1:90:A:GLU:HA   | 1:84:A:ARG:HA   | 6                   | 0.12     | 0.02                | 0.12       |
| (3,2949) | 1:90:A:GLU:HA   | 1:84:A:ARG:HA   | 6                   | 0.12     | 0.02                | 0.12       |
| (1,1502) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD11 | 6                   | 0.12     | 0.02                | 0.11       |
| (1,1502) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD12 | 6                   | 0.12     | 0.02                | 0.11       |
| (1,1502) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD13 | 6                   | 0.12     | 0.02                | 0.11       |
| (1,1502) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD11 | 6                   | 0.12     | 0.02                | 0.11       |
| (1,1502) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD12 | 6                   | 0.12     | 0.02                | 0.11       |
| (1,1502) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD13 | 6                   | 0.12     | 0.02                | 0.11       |
| (1,1502) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD11 | 6                   | 0.12     | 0.02                | 0.11       |
| (1,1502) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD12 | 6                   | 0.12     | 0.02                | 0.11       |
| (1,1502) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD13 | 6                   | 0.12     | 0.02                | 0.11       |
| (1,1903) | 1:66:A:MET:HE1  | 1:79:A:TYR:HA   | 6                   | 0.12     | 0.02                | 0.11       |
| (1,1903) | 1:66:A:MET:HE2  | 1:79:A:TYR:HA   | 6                   | 0.12     | 0.02                | 0.11       |
| (1,1903) | 1:66:A:MET:HE3  | 1:79:A:TYR:HA   | 6                   | 0.12     | 0.02                | 0.11       |
| (1,1994) | 1:21:A:VAL:HG11 | 1:25:A:GLN:HG3  | 6                   | 0.12     | 0.01                | 0.11       |
| (1,1994) | 1:21:A:VAL:HG12 | 1:25:A:GLN:HG3  | 6                   | 0.12     | 0.01                | 0.11       |
| (1,1994) | 1:21:A:VAL:HG13 | 1:25:A:GLN:HG3  | 6                   | 0.12     | 0.01                | 0.11       |
| (3,1506) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD11 | 6                   | 0.12     | 0.02                | 0.11       |
| (3,1506) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD12 | 6                   | 0.12     | 0.02                | 0.11       |
| (3,1506) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD13 | 6                   | 0.12     | 0.02                | 0.11       |
| (3,1506) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD11 | 6                   | 0.12     | 0.02                | 0.11       |
| (3,1506) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD12 | 6                   | 0.12     | 0.02                | 0.11       |
| (3,1506) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD13 | 6                   | 0.12     | 0.02                | 0.11       |
| (3,1506) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD11 | 6                   | 0.12     | 0.02                | 0.11       |
| (3,1506) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD12 | 6                   | 0.12     | 0.02                | 0.11       |
| (3,1506) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD13 | 6                   | 0.12     | 0.02                | 0.11       |
| (3,1906) | 1:66:A:MET:HE1  | 1:79:A:TYR:HA   | 6                   | 0.12     | 0.02                | 0.11       |
| (3,1906) | 1:66:A:MET:HE2  | 1:79:A:TYR:HA   | 6                   | 0.12     | 0.02                | 0.11       |
| (3,1906) | 1:66:A:MET:HE3  | 1:79:A:TYR:HA   | 6                   | 0.12     | 0.02                | 0.11       |
| (3,1997) | 1:21:A:VAL:HG11 | 1:25:A:GLN:HG3  | 6                   | 0.12     | 0.01                | 0.11       |
| (3,1997) | 1:21:A:VAL:HG12 | 1:25:A:GLN:HG3  | 6                   | 0.12     | 0.01                | 0.11       |
| (3,1997) | 1:21:A:VAL:HG13 | 1:25:A:GLN:HG3  | 6                   | 0.12     | 0.01                | 0.11       |
| (1,1204) | 1:42:A:TRP:H    | 1:57:A:PHE:HE1  | 6                   | 0.11     | 0.01                | 0.11       |
| (1,1204) | 1:42:A:TRP:H    | 1:57:A:PHE:HE2  | 6                   | 0.11     | 0.01                | 0.11       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (3,1208) | 1:42:A:TRP:H    | 1:57:A:PHE:HE1  | 6                   | 0.11     | 0.01                | 0.11       |
| (3,1208) | 1:42:A:TRP:H    | 1:57:A:PHE:HE2  | 6                   | 0.11     | 0.01                | 0.11       |
| (1,1208) | 1:56:A:ASN:H    | 1:66:A:MET:HG2  | 6                   | 0.11     | 0.01                | 0.11       |
| (3,1212) | 1:56:A:ASN:H    | 1:66:A:MET:HG2  | 6                   | 0.11     | 0.01                | 0.11       |
| (1,826)  | 1:17:A:GLN:H    | 1:17:A:GLN:HG2  | 5                   | 0.24     | 0.01                | 0.24       |
| (3,826)  | 1:17:A:GLN:H    | 1:17:A:GLN:HG2  | 5                   | 0.24     | 0.01                | 0.24       |
| (1,3199) | 1:43:A:TYR:HD1  | 1:80:A:SER:HB2  | 5                   | 0.19     | 0.04                | 0.18       |
| (1,3199) | 1:43:A:TYR:HD2  | 1:80:A:SER:HB2  | 5                   | 0.19     | 0.04                | 0.18       |
| (3,3205) | 1:43:A:TYR:HD1  | 1:80:A:SER:HB2  | 5                   | 0.19     | 0.04                | 0.18       |
| (3,3205) | 1:43:A:TYR:HD2  | 1:80:A:SER:HB2  | 5                   | 0.19     | 0.04                | 0.18       |
| (1,1177) | 1:100:A:GLU:H   | 1:21:A:VAL:HG11 | 5                   | 0.16     | 0.02                | 0.16       |
| (1,1177) | 1:100:A:GLU:H   | 1:21:A:VAL:HG12 | 5                   | 0.16     | 0.02                | 0.16       |
| (1,1177) | 1:100:A:GLU:H   | 1:21:A:VAL:HG13 | 5                   | 0.16     | 0.02                | 0.16       |
| (3,1181) | 1:100:A:GLU:H   | 1:21:A:VAL:HG11 | 5                   | 0.16     | 0.02                | 0.16       |
| (3,1181) | 1:100:A:GLU:H   | 1:21:A:VAL:HG12 | 5                   | 0.16     | 0.02                | 0.16       |
| (3,1181) | 1:100:A:GLU:H   | 1:21:A:VAL:HG13 | 5                   | 0.16     | 0.02                | 0.16       |
| (1,368)  | 1:18:A:ASN:H    | 1:17:A:GLN:HB3  | 5                   | 0.15     | 0.01                | 0.15       |
| (3,368)  | 1:18:A:ASN:H    | 1:17:A:GLN:HB3  | 5                   | 0.15     | 0.01                | 0.15       |
| (1,591)  | 1:3:A:ASP:H     | 1:3:A:ASP:HA    | 5                   | 0.15     | 0.01                | 0.15       |
| (3,591)  | 1:3:A:ASP:H     | 1:3:A:ASP:HA    | 5                   | 0.15     | 0.01                | 0.15       |
| (1,410)  | 1:96:A:GLU:H    | 1:18:A:ASN:HD21 | 5                   | 0.14     | 0.03                | 0.14       |
| (3,410)  | 1:96:A:GLU:H    | 1:18:A:ASN:HD21 | 5                   | 0.14     | 0.03                | 0.14       |
| (1,2929) | 1:17:A:GLN:HG2  | 1:17:A:GLN:H    | 5                   | 0.14     | 0.01                | 0.14       |
| (3,2936) | 1:17:A:GLN:HG2  | 1:17:A:GLN:H    | 5                   | 0.14     | 0.01                | 0.14       |
| (1,25)   | 1:89:A:GLY:H    | 1:88:A:ARG:HB3  | 5                   | 0.14     | 0.02                | 0.13       |
| (3,25)   | 1:89:A:GLY:H    | 1:88:A:ARG:HB3  | 5                   | 0.14     | 0.02                | 0.13       |
| (1,1679) | 1:85:A:LEU:HD11 | 1:35:A:PHE:HD1  | 5                   | 0.13     | 0.02                | 0.13       |
| (1,1679) | 1:85:A:LEU:HD11 | 1:35:A:PHE:HD2  | 5                   | 0.13     | 0.02                | 0.13       |
| (1,1679) | 1:85:A:LEU:HD12 | 1:35:A:PHE:HD1  | 5                   | 0.13     | 0.02                | 0.13       |
| (1,1679) | 1:85:A:LEU:HD12 | 1:35:A:PHE:HD2  | 5                   | 0.13     | 0.02                | 0.13       |
| (1,1679) | 1:85:A:LEU:HD13 | 1:35:A:PHE:HD1  | 5                   | 0.13     | 0.02                | 0.13       |
| (1,1679) | 1:85:A:LEU:HD13 | 1:35:A:PHE:HD2  | 5                   | 0.13     | 0.02                | 0.13       |
| (3,1683) | 1:85:A:LEU:HD11 | 1:35:A:PHE:HD1  | 5                   | 0.13     | 0.02                | 0.13       |
| (3,1683) | 1:85:A:LEU:HD11 | 1:35:A:PHE:HD2  | 5                   | 0.13     | 0.02                | 0.13       |
| (3,1683) | 1:85:A:LEU:HD12 | 1:35:A:PHE:HD1  | 5                   | 0.13     | 0.02                | 0.13       |
| (3,1683) | 1:85:A:LEU:HD12 | 1:35:A:PHE:HD2  | 5                   | 0.13     | 0.02                | 0.13       |
| (3,1683) | 1:85:A:LEU:HD13 | 1:35:A:PHE:HD1  | 5                   | 0.13     | 0.02                | 0.13       |
| (3,1683) | 1:85:A:LEU:HD13 | 1:35:A:PHE:HD2  | 5                   | 0.13     | 0.02                | 0.13       |
| (1,404)  | 1:77:A:GLY:H    | 1:97:A:LEU:HD21 | 5                   | 0.13     | 0.01                | 0.13       |
| (1,404)  | 1:77:A:GLY:H    | 1:97:A:LEU:HD22 | 5                   | 0.13     | 0.01                | 0.13       |
| (1,404)  | 1:77:A:GLY:H    | 1:97:A:LEU:HD23 | 5                   | 0.13     | 0.01                | 0.13       |
| (1,1289) | 1:40:A:VAL:HG21 | 1:42:A:TRP:HE1  | 5                   | 0.13     | 0.01                | 0.13       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1289) | 1:40:A:VAL:HG22 | 1:42:A:TRP:HE1  | 5                   | 0.13     | 0.01                | 0.13       |
| (1,1289) | 1:40:A:VAL:HG23 | 1:42:A:TRP:HE1  | 5                   | 0.13     | 0.01                | 0.13       |
| (3,404)  | 1:77:A:GLY:H    | 1:97:A:LEU:HD21 | 5                   | 0.13     | 0.01                | 0.13       |
| (3,404)  | 1:77:A:GLY:H    | 1:97:A:LEU:HD22 | 5                   | 0.13     | 0.01                | 0.13       |
| (3,404)  | 1:77:A:GLY:H    | 1:97:A:LEU:HD23 | 5                   | 0.13     | 0.01                | 0.13       |
| (3,1293) | 1:40:A:VAL:HG21 | 1:42:A:TRP:HE1  | 5                   | 0.13     | 0.01                | 0.13       |
| (3,1293) | 1:40:A:VAL:HG22 | 1:42:A:TRP:HE1  | 5                   | 0.13     | 0.01                | 0.13       |
| (3,1293) | 1:40:A:VAL:HG23 | 1:42:A:TRP:HE1  | 5                   | 0.13     | 0.01                | 0.13       |
| (1,393)  | 1:77:A:GLY:H    | 1:96:A:GLU:HA   | 5                   | 0.12     | 0.02                | 0.12       |
| (1,1952) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB1  | 5                   | 0.12     | 0.02                | 0.12       |
| (1,1952) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB2  | 5                   | 0.12     | 0.02                | 0.12       |
| (1,1952) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB3  | 5                   | 0.12     | 0.02                | 0.12       |
| (1,1952) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB1  | 5                   | 0.12     | 0.02                | 0.12       |
| (1,1952) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB2  | 5                   | 0.12     | 0.02                | 0.12       |
| (1,1952) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB3  | 5                   | 0.12     | 0.02                | 0.12       |
| (1,1952) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB1  | 5                   | 0.12     | 0.02                | 0.12       |
| (1,1952) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB2  | 5                   | 0.12     | 0.02                | 0.12       |
| (1,1952) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB3  | 5                   | 0.12     | 0.02                | 0.12       |
| (3,393)  | 1:77:A:GLY:H    | 1:96:A:GLU:HA   | 5                   | 0.12     | 0.02                | 0.12       |
| (3,1955) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB1  | 5                   | 0.12     | 0.02                | 0.12       |
| (3,1955) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB2  | 5                   | 0.12     | 0.02                | 0.12       |
| (3,1955) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB3  | 5                   | 0.12     | 0.02                | 0.12       |
| (3,1955) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB1  | 5                   | 0.12     | 0.02                | 0.12       |
| (3,1955) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB2  | 5                   | 0.12     | 0.02                | 0.12       |
| (3,1955) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB3  | 5                   | 0.12     | 0.02                | 0.12       |
| (3,1955) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB1  | 5                   | 0.12     | 0.02                | 0.12       |
| (3,1955) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB2  | 5                   | 0.12     | 0.02                | 0.12       |
| (3,1955) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB3  | 5                   | 0.12     | 0.02                | 0.12       |
| (1,2070) | 1:97:A:LEU:HB2  | 1:19:A:ILE:HB   | 5                   | 0.12     | 0.03                | 0.11       |
| (3,2075) | 1:97:A:LEU:HB2  | 1:19:A:ILE:HB   | 5                   | 0.12     | 0.03                | 0.11       |
| (1,1650) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,1650) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,1650) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,1650) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,1650) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,1650) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,1650) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,1650) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,1650) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 5                   | 0.11     | 0.01                | 0.11       |
| (3,1654) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 5                   | 0.11     | 0.01                | 0.11       |
| (3,1654) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 5                   | 0.11     | 0.01                | 0.11       |
| (3,1654) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 5                   | 0.11     | 0.01                | 0.11       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (3,1654) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 5                   | 0.11     | 0.01                | 0.11       |
| (3,1654) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 5                   | 0.11     | 0.01                | 0.11       |
| (3,1654) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 5                   | 0.11     | 0.01                | 0.11       |
| (3,1654) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 5                   | 0.11     | 0.01                | 0.11       |
| (3,1654) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 5                   | 0.11     | 0.01                | 0.11       |
| (3,1654) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,3009) | 1:102:A:ARG:HD3 | 1:102:A:ARG:HB2 | 5                   | 0.11     | 0.01                | 0.11       |
| (3,3017) | 1:102:A:ARG:HD3 | 1:102:A:ARG:HB2 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,1536) | 1:39:A:ILE:HD11 | 1:40:A:VAL:H    | 4                   | 0.23     | 0.01                | 0.22       |
| (1,1536) | 1:39:A:ILE:HD12 | 1:40:A:VAL:H    | 4                   | 0.23     | 0.01                | 0.22       |
| (1,1536) | 1:39:A:ILE:HD13 | 1:40:A:VAL:H    | 4                   | 0.23     | 0.01                | 0.22       |
| (3,1540) | 1:39:A:ILE:HD11 | 1:40:A:VAL:H    | 4                   | 0.23     | 0.01                | 0.22       |
| (3,1540) | 1:39:A:ILE:HD12 | 1:40:A:VAL:H    | 4                   | 0.23     | 0.01                | 0.22       |
| (3,1540) | 1:39:A:ILE:HD13 | 1:40:A:VAL:H    | 4                   | 0.23     | 0.01                | 0.22       |
| (1,786)  | 1:6:A:THR:H     | 1:6:A:THR:HG21  | 4                   | 0.18     | 0.02                | 0.18       |
| (1,786)  | 1:6:A:THR:H     | 1:6:A:THR:HG22  | 4                   | 0.18     | 0.02                | 0.18       |
| (1,786)  | 1:6:A:THR:H     | 1:6:A:THR:HG23  | 4                   | 0.18     | 0.02                | 0.18       |
| (3,786)  | 1:6:A:THR:H     | 1:6:A:THR:HG21  | 4                   | 0.18     | 0.02                | 0.18       |
| (3,786)  | 1:6:A:THR:H     | 1:6:A:THR:HG22  | 4                   | 0.18     | 0.02                | 0.18       |
| (3,786)  | 1:6:A:THR:H     | 1:6:A:THR:HG23  | 4                   | 0.18     | 0.02                | 0.18       |
| (1,22)   | 1:89:A:GLY:H    | 1:85:A:LEU:H    | 4                   | 0.17     | 0.02                | 0.16       |
| (1,2076) | 1:97:A:LEU:HD11 | 1:21:A:VAL:HB   | 4                   | 0.14     | 0.03                | 0.13       |
| (1,2076) | 1:97:A:LEU:HD12 | 1:21:A:VAL:HB   | 4                   | 0.14     | 0.03                | 0.13       |
| (1,2076) | 1:97:A:LEU:HD13 | 1:21:A:VAL:HB   | 4                   | 0.14     | 0.03                | 0.13       |
| (3,2081) | 1:97:A:LEU:HD11 | 1:21:A:VAL:HB   | 4                   | 0.14     | 0.03                | 0.13       |
| (3,2081) | 1:97:A:LEU:HD12 | 1:21:A:VAL:HB   | 4                   | 0.14     | 0.03                | 0.13       |
| (3,2081) | 1:97:A:LEU:HD13 | 1:21:A:VAL:HB   | 4                   | 0.14     | 0.03                | 0.13       |
| (1,314)  | 1:63:A:CYS:H    | 1:64:A:HIS:HD2  | 4                   | 0.13     | 0.03                | 0.13       |
| (1,1064) | 1:71:A:VAL:H    | 1:25:A:GLN:H    | 4                   | 0.13     | 0.02                | 0.12       |
| (3,314)  | 1:63:A:CYS:H    | 1:64:A:HIS:HD2  | 4                   | 0.13     | 0.03                | 0.13       |
| (3,1063) | 1:71:A:VAL:H    | 1:25:A:GLN:H    | 4                   | 0.13     | 0.02                | 0.12       |
| (1,2068) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 4                   | 0.13     | 0.01                | 0.12       |
| (1,2068) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 4                   | 0.13     | 0.01                | 0.12       |
| (1,2068) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 4                   | 0.13     | 0.01                | 0.12       |
| (3,2073) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 4                   | 0.13     | 0.01                | 0.12       |
| (3,2073) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 4                   | 0.13     | 0.01                | 0.12       |
| (3,2073) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 4                   | 0.13     | 0.01                | 0.12       |
| (1,1956) | 1:72:A:THR:HG21 | 1:74:A:ASP:HB3  | 4                   | 0.12     | 0.02                | 0.12       |
| (1,1956) | 1:72:A:THR:HG22 | 1:74:A:ASP:HB3  | 4                   | 0.12     | 0.02                | 0.12       |
| (1,1956) | 1:72:A:THR:HG23 | 1:74:A:ASP:HB3  | 4                   | 0.12     | 0.02                | 0.12       |
| (1,2093) | 1:88:A:ARG:HD3  | 1:7:A:ALA:HA    | 4                   | 0.12     | 0.01                | 0.12       |
| (1,2339) | 1:26:A:SER:HB3  | 1:27:A:ALA:H    | 4                   | 0.12     | 0.01                | 0.12       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (3,1959) | 1:72:A:THR:HG21 | 1:74:A:ASP:HB3  | 4                   | 0.12     | 0.02                | 0.12       |
| (3,1959) | 1:72:A:THR:HG22 | 1:74:A:ASP:HB3  | 4                   | 0.12     | 0.02                | 0.12       |
| (3,1959) | 1:72:A:THR:HG23 | 1:74:A:ASP:HB3  | 4                   | 0.12     | 0.02                | 0.12       |
| (3,2342) | 1:26:A:SER:HB3  | 1:27:A:ALA:H    | 4                   | 0.12     | 0.01                | 0.12       |
| (3,3092) | 1:7:A:ALA:HB1   | 1:88:A:ARG:HD3  | 4                   | 0.12     | 0.01                | 0.12       |
| (3,3092) | 1:7:A:ALA:HB2   | 1:88:A:ARG:HD3  | 4                   | 0.12     | 0.01                | 0.12       |
| (3,3092) | 1:7:A:ALA:HB3   | 1:88:A:ARG:HD3  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,915)  | 1:37:A:ASP:H    | 1:37:A:ASP:HA   | 4                   | 0.12     | 0.01                | 0.12       |
| (3,916)  | 1:37:A:ASP:H    | 1:37:A:ASP:HA   | 4                   | 0.12     | 0.01                | 0.12       |
| (1,2715) | 1:48:A:GLU:HA   | 1:49:A:LEU:HG   | 4                   | 0.11     | 0.02                | 0.11       |
| (3,2719) | 1:48:A:GLU:HA   | 1:49:A:LEU:HG   | 4                   | 0.11     | 0.02                | 0.11       |
| (1,182)  | 1:11:A:GLN:H    | 1:10:A:ILE:HD11 | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,182)  | 1:11:A:GLN:H    | 1:10:A:ILE:HD12 | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,182)  | 1:11:A:GLN:H    | 1:10:A:ILE:HD13 | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,1622) | 1:82:A:ILE:HD11 | 1:83:A:ALA:H    | 4                   | 0.11     | 0.01                | 0.11       |
| (1,1622) | 1:82:A:ILE:HD12 | 1:83:A:ALA:H    | 4                   | 0.11     | 0.01                | 0.11       |
| (1,1622) | 1:82:A:ILE:HD13 | 1:83:A:ALA:H    | 4                   | 0.11     | 0.01                | 0.11       |
| (3,182)  | 1:11:A:GLN:H    | 1:10:A:ILE:HD11 | 4                   | 0.11     | 0.0                 | 0.11       |
| (3,182)  | 1:11:A:GLN:H    | 1:10:A:ILE:HD12 | 4                   | 0.11     | 0.0                 | 0.11       |
| (3,182)  | 1:11:A:GLN:H    | 1:10:A:ILE:HD13 | 4                   | 0.11     | 0.0                 | 0.11       |
| (3,1626) | 1:82:A:ILE:HD11 | 1:83:A:ALA:H    | 4                   | 0.11     | 0.01                | 0.11       |
| (3,1626) | 1:82:A:ILE:HD12 | 1:83:A:ALA:H    | 4                   | 0.11     | 0.01                | 0.11       |
| (3,1626) | 1:82:A:ILE:HD13 | 1:83:A:ALA:H    | 4                   | 0.11     | 0.01                | 0.11       |
| (1,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HG3  | 4                   | 0.11     | 0.0                 | 0.11       |
| (3,2917) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HG3  | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,2716) | 1:48:A:GLU:HA   | 1:41:A:THR:HG21 | 4                   | 0.1      | 0.0                 | 0.1        |
| (1,2716) | 1:48:A:GLU:HA   | 1:41:A:THR:HG22 | 4                   | 0.1      | 0.0                 | 0.1        |
| (1,2716) | 1:48:A:GLU:HA   | 1:41:A:THR:HG23 | 4                   | 0.1      | 0.0                 | 0.1        |
| (3,2720) | 1:48:A:GLU:HA   | 1:41:A:THR:HG21 | 4                   | 0.1      | 0.0                 | 0.1        |
| (3,2720) | 1:48:A:GLU:HA   | 1:41:A:THR:HG22 | 4                   | 0.1      | 0.0                 | 0.1        |
| (3,2720) | 1:48:A:GLU:HA   | 1:41:A:THR:HG23 | 4                   | 0.1      | 0.0                 | 0.1        |
| (3,1241) | 1:13:A:THR:HG21 | 1:34:A:SER:HB2  | 3                   | 0.44     | 0.02                | 0.44       |
| (3,1241) | 1:13:A:THR:HG22 | 1:34:A:SER:HB2  | 3                   | 0.44     | 0.02                | 0.44       |
| (3,1241) | 1:13:A:THR:HG23 | 1:34:A:SER:HB2  | 3                   | 0.44     | 0.02                | 0.44       |
| (1,1237) | 1:13:A:THR:HG21 | 1:34:A:SER:HB2  | 3                   | 0.24     | 0.02                | 0.24       |
| (1,1237) | 1:13:A:THR:HG22 | 1:34:A:SER:HB2  | 3                   | 0.24     | 0.02                | 0.24       |
| (1,1237) | 1:13:A:THR:HG23 | 1:34:A:SER:HB2  | 3                   | 0.24     | 0.02                | 0.24       |
| (1,2961) | 1:44:A:LYS:HE2  | 1:44:A:LYS:HG2  | 3                   | 0.22     | 0.0                 | 0.22       |
| (3,2969) | 1:44:A:LYS:HE2  | 1:44:A:LYS:HG2  | 3                   | 0.22     | 0.0                 | 0.22       |
| (1,1535) | 1:2:A:ILE:HD11  | 1:2:A:ILE:HA    | 3                   | 0.21     | 0.06                | 0.2        |
| (1,1535) | 1:2:A:ILE:HD12  | 1:2:A:ILE:HA    | 3                   | 0.21     | 0.06                | 0.2        |
| (1,1535) | 1:2:A:ILE:HD13  | 1:2:A:ILE:HA    | 3                   | 0.21     | 0.06                | 0.2        |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (3,1539) | 1:2:A:ILE:HD11  | 1:2:A:ILE:HA    | 3                   | 0.21     | 0.06                | 0.2        |
| (3,1539) | 1:2:A:ILE:HD12  | 1:2:A:ILE:HA    | 3                   | 0.21     | 0.06                | 0.2        |
| (3,1539) | 1:2:A:ILE:HD13  | 1:2:A:ILE:HA    | 3                   | 0.21     | 0.06                | 0.2        |
| (1,1125) | 1:78:A:VAL:H    | 1:44:A:LYS:HE2  | 3                   | 0.15     | 0.02                | 0.16       |
| (3,1126) | 1:78:A:VAL:H    | 1:44:A:LYS:HE2  | 3                   | 0.15     | 0.02                | 0.16       |
| (1,2962) | 1:44:A:LYS:HE2  | 1:44:A:LYS:HG3  | 3                   | 0.15     | 0.01                | 0.15       |
| (3,2970) | 1:44:A:LYS:HE2  | 1:44:A:LYS:HG3  | 3                   | 0.15     | 0.01                | 0.15       |
| (1,142)  | 1:101:A:LEU:H   | 1:100:A:GLU:HB2 | 3                   | 0.14     | 0.02                | 0.15       |
| (3,144)  | 1:101:A:LEU:H   | 1:100:A:GLU:HB2 | 3                   | 0.14     | 0.02                | 0.15       |
| (1,2967) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD2  | 3                   | 0.13     | 0.0                 | 0.13       |
| (3,2975) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD2  | 3                   | 0.13     | 0.0                 | 0.13       |
| (1,2930) | 1:17:A:GLN:HG2  | 1:18:A:ASN:H    | 3                   | 0.12     | 0.03                | 0.1        |
| (3,2937) | 1:17:A:GLN:HG2  | 1:18:A:ASN:H    | 3                   | 0.12     | 0.03                | 0.1        |
| (1,1408) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HA  | 3                   | 0.12     | 0.01                | 0.12       |
| (1,1408) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HA  | 3                   | 0.12     | 0.01                | 0.12       |
| (1,1408) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HA  | 3                   | 0.12     | 0.01                | 0.12       |
| (3,1412) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HA  | 3                   | 0.12     | 0.01                | 0.12       |
| (3,1412) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HA  | 3                   | 0.12     | 0.01                | 0.12       |
| (3,1412) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HA  | 3                   | 0.12     | 0.01                | 0.12       |
| (1,1420) | 1:21:A:VAL:HG21 | 1:19:A:ILE:HD11 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1420) | 1:21:A:VAL:HG21 | 1:19:A:ILE:HD12 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1420) | 1:21:A:VAL:HG21 | 1:19:A:ILE:HD13 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1420) | 1:21:A:VAL:HG22 | 1:19:A:ILE:HD11 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1420) | 1:21:A:VAL:HG22 | 1:19:A:ILE:HD12 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1420) | 1:21:A:VAL:HG22 | 1:19:A:ILE:HD13 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1420) | 1:21:A:VAL:HG23 | 1:19:A:ILE:HD11 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1420) | 1:21:A:VAL:HG23 | 1:19:A:ILE:HD12 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1420) | 1:21:A:VAL:HG23 | 1:19:A:ILE:HD13 | 3                   | 0.11     | 0.0                 | 0.11       |
| (3,1424) | 1:21:A:VAL:HG21 | 1:19:A:ILE:HD11 | 3                   | 0.11     | 0.0                 | 0.11       |
| (3,1424) | 1:21:A:VAL:HG21 | 1:19:A:ILE:HD12 | 3                   | 0.11     | 0.0                 | 0.11       |
| (3,1424) | 1:21:A:VAL:HG21 | 1:19:A:ILE:HD13 | 3                   | 0.11     | 0.0                 | 0.11       |
| (3,1424) | 1:21:A:VAL:HG22 | 1:19:A:ILE:HD11 | 3                   | 0.11     | 0.0                 | 0.11       |
| (3,1424) | 1:21:A:VAL:HG22 | 1:19:A:ILE:HD12 | 3                   | 0.11     | 0.0                 | 0.11       |
| (3,1424) | 1:21:A:VAL:HG22 | 1:19:A:ILE:HD13 | 3                   | 0.11     | 0.0                 | 0.11       |
| (3,1424) | 1:21:A:VAL:HG23 | 1:19:A:ILE:HD11 | 3                   | 0.11     | 0.0                 | 0.11       |
| (3,1424) | 1:21:A:VAL:HG23 | 1:19:A:ILE:HD12 | 3                   | 0.11     | 0.0                 | 0.11       |
| (3,1424) | 1:21:A:VAL:HG23 | 1:19:A:ILE:HD13 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1548) | 1:10:A:ILE:HG21 | 1:83:A:ALA:HB1  | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1548) | 1:10:A:ILE:HG21 | 1:83:A:ALA:HB2  | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1548) | 1:10:A:ILE:HG21 | 1:83:A:ALA:HB3  | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1548) | 1:10:A:ILE:HG22 | 1:83:A:ALA:HB1  | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1548) | 1:10:A:ILE:HG22 | 1:83:A:ALA:HB2  | 3                   | 0.11     | 0.0                 | 0.11       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1548) | 1:10:A:ILE:HG22  | 1:83:A:ALA:HB3  | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1548) | 1:10:A:ILE:HG23  | 1:83:A:ALA:HB1  | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1548) | 1:10:A:ILE:HG23  | 1:83:A:ALA:HB2  | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1548) | 1:10:A:ILE:HG23  | 1:83:A:ALA:HB3  | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1654) | 1:40:A:VAL:HB    | 1:39:A:ILE:HA   | 3                   | 0.11     | 0.0                 | 0.11       |
| (3,1552) | 1:10:A:ILE:HG21  | 1:83:A:ALA:HB1  | 3                   | 0.11     | 0.0                 | 0.11       |
| (3,1552) | 1:10:A:ILE:HG21  | 1:83:A:ALA:HB2  | 3                   | 0.11     | 0.0                 | 0.11       |
| (3,1552) | 1:10:A:ILE:HG21  | 1:83:A:ALA:HB3  | 3                   | 0.11     | 0.0                 | 0.11       |
| (3,1552) | 1:10:A:ILE:HG22  | 1:83:A:ALA:HB1  | 3                   | 0.11     | 0.0                 | 0.11       |
| (3,1552) | 1:10:A:ILE:HG22  | 1:83:A:ALA:HB2  | 3                   | 0.11     | 0.0                 | 0.11       |
| (3,1552) | 1:10:A:ILE:HG22  | 1:83:A:ALA:HB3  | 3                   | 0.11     | 0.0                 | 0.11       |
| (3,1552) | 1:10:A:ILE:HG23  | 1:83:A:ALA:HB1  | 3                   | 0.11     | 0.0                 | 0.11       |
| (3,1552) | 1:10:A:ILE:HG23  | 1:83:A:ALA:HB2  | 3                   | 0.11     | 0.0                 | 0.11       |
| (3,1552) | 1:10:A:ILE:HG23  | 1:83:A:ALA:HB3  | 3                   | 0.11     | 0.0                 | 0.11       |
| (3,1658) | 1:40:A:VAL:HB    | 1:39:A:ILE:HA   | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1696) | 1:101:A:LEU:HD21 | 1:101:A:LEU:HB3 | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,1696) | 1:101:A:LEU:HD22 | 1:101:A:LEU:HB3 | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,1696) | 1:101:A:LEU:HD23 | 1:101:A:LEU:HB3 | 3                   | 0.1      | 0.0                 | 0.1        |
| (3,1700) | 1:101:A:LEU:HD21 | 1:101:A:LEU:HB3 | 3                   | 0.1      | 0.0                 | 0.1        |
| (3,1700) | 1:101:A:LEU:HD22 | 1:101:A:LEU:HB3 | 3                   | 0.1      | 0.0                 | 0.1        |
| (3,1700) | 1:101:A:LEU:HD23 | 1:101:A:LEU:HB3 | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,2672) | 1:25:A:GLN:HG3   | 1:22:A:SER:HB2  | 2                   | 0.26     | 0.03                | 0.26       |
| (3,2676) | 1:25:A:GLN:HG3   | 1:22:A:SER:HB2  | 2                   | 0.26     | 0.03                | 0.26       |
| (1,2916) | 1:22:A:SER:HB2   | 1:22:A:SER:H    | 2                   | 0.24     | 0.0                 | 0.24       |
| (3,2923) | 1:22:A:SER:HB2   | 1:22:A:SER:H    | 2                   | 0.24     | 0.0                 | 0.24       |
| (1,669)  | 1:72:A:THR:H     | 1:72:A:THR:HG21 | 2                   | 0.2      | 0.01                | 0.2        |
| (1,669)  | 1:72:A:THR:H     | 1:72:A:THR:HG22 | 2                   | 0.2      | 0.01                | 0.2        |
| (1,669)  | 1:72:A:THR:H     | 1:72:A:THR:HG23 | 2                   | 0.2      | 0.01                | 0.2        |
| (1,2613) | 1:74:A:ASP:HB2   | 1:74:A:ASP:HA   | 2                   | 0.2      | 0.01                | 0.2        |
| (3,669)  | 1:72:A:THR:H     | 1:72:A:THR:HG21 | 2                   | 0.2      | 0.01                | 0.2        |
| (3,669)  | 1:72:A:THR:H     | 1:72:A:THR:HG22 | 2                   | 0.2      | 0.01                | 0.2        |
| (3,669)  | 1:72:A:THR:H     | 1:72:A:THR:HG23 | 2                   | 0.2      | 0.01                | 0.2        |
| (3,2617) | 1:74:A:ASP:HB2   | 1:74:A:ASP:HA   | 2                   | 0.2      | 0.01                | 0.2        |
| (1,783)  | 1:74:A:ASP:H     | 1:74:A:ASP:HB3  | 2                   | 0.18     | 0.0                 | 0.18       |
| (1,2215) | 1:56:A:ASN:HA    | 1:56:A:ASN:HD21 | 2                   | 0.18     | 0.02                | 0.18       |
| (1,2615) | 1:74:A:ASP:HB3   | 1:74:A:ASP:H    | 2                   | 0.18     | 0.0                 | 0.18       |
| (3,783)  | 1:74:A:ASP:H     | 1:74:A:ASP:HB3  | 2                   | 0.18     | 0.0                 | 0.18       |
| (3,2218) | 1:56:A:ASN:HA    | 1:56:A:ASN:HD21 | 2                   | 0.18     | 0.02                | 0.18       |
| (3,2619) | 1:74:A:ASP:HB3   | 1:74:A:ASP:H    | 2                   | 0.18     | 0.0                 | 0.18       |
| (1,136)  | 1:39:A:ILE:H     | 1:10:A:ILE:HD11 | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,136)  | 1:39:A:ILE:H     | 1:10:A:ILE:HD12 | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,136)  | 1:39:A:ILE:H     | 1:10:A:ILE:HD13 | 2                   | 0.14     | 0.0                 | 0.14       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1043) | 1:26:A:SER:H    | 1:26:A:SER:HB3  | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,1966) | 1:36:A:ASP:HB3  | 1:62:A:ARG:HA   | 2                   | 0.14     | 0.02                | 0.14       |
| (3,138)  | 1:39:A:ILE:H    | 1:10:A:ILE:HD11 | 2                   | 0.14     | 0.0                 | 0.14       |
| (3,138)  | 1:39:A:ILE:H    | 1:10:A:ILE:HD12 | 2                   | 0.14     | 0.0                 | 0.14       |
| (3,138)  | 1:39:A:ILE:H    | 1:10:A:ILE:HD13 | 2                   | 0.14     | 0.0                 | 0.14       |
| (3,1042) | 1:26:A:SER:H    | 1:26:A:SER:HB3  | 2                   | 0.14     | 0.0                 | 0.14       |
| (3,1969) | 1:36:A:ASP:HB3  | 1:62:A:ARG:HA   | 2                   | 0.14     | 0.02                | 0.14       |
| (1,672)  | 1:72:A:THR:H    | 1:73:A:PRO:HD2  | 2                   | 0.14     | 0.02                | 0.14       |
| (1,2136) | 1:67:A:THR:HB   | 1:56:A:ASN:HB2  | 2                   | 0.14     | 0.01                | 0.14       |
| (3,672)  | 1:72:A:THR:H    | 1:73:A:PRO:HD2  | 2                   | 0.14     | 0.02                | 0.14       |
| (3,2139) | 1:67:A:THR:HB   | 1:56:A:ASN:HB2  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,683)  | 1:23:A:GLU:H    | 1:22:A:SER:HB3  | 2                   | 0.13     | 0.01                | 0.13       |
| (3,683)  | 1:23:A:GLU:H    | 1:22:A:SER:HB3  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,875)  | 1:8:A:GLU:H     | 1:7:A:ALA:HB1   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,875)  | 1:8:A:GLU:H     | 1:7:A:ALA:HB2   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,875)  | 1:8:A:GLU:H     | 1:7:A:ALA:HB3   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1248) | 1:28:A:THR:HG21 | 1:67:A:THR:HG21 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1248) | 1:28:A:THR:HG21 | 1:67:A:THR:HG22 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1248) | 1:28:A:THR:HG21 | 1:67:A:THR:HG23 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1248) | 1:28:A:THR:HG22 | 1:67:A:THR:HG21 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1248) | 1:28:A:THR:HG22 | 1:67:A:THR:HG22 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1248) | 1:28:A:THR:HG22 | 1:67:A:THR:HG23 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1248) | 1:28:A:THR:HG23 | 1:67:A:THR:HG21 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1248) | 1:28:A:THR:HG23 | 1:67:A:THR:HG22 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1248) | 1:28:A:THR:HG23 | 1:67:A:THR:HG23 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1863) | 1:7:A:ALA:HB1   | 1:8:A:GLU:H     | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1863) | 1:7:A:ALA:HB2   | 1:8:A:GLU:H     | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1863) | 1:7:A:ALA:HB3   | 1:8:A:GLU:H     | 2                   | 0.12     | 0.02                | 0.12       |
| (3,875)  | 1:8:A:GLU:H     | 1:7:A:ALA:HB1   | 2                   | 0.12     | 0.02                | 0.12       |
| (3,875)  | 1:8:A:GLU:H     | 1:7:A:ALA:HB2   | 2                   | 0.12     | 0.02                | 0.12       |
| (3,875)  | 1:8:A:GLU:H     | 1:7:A:ALA:HB3   | 2                   | 0.12     | 0.02                | 0.12       |
| (3,1252) | 1:28:A:THR:HG21 | 1:67:A:THR:HG21 | 2                   | 0.12     | 0.02                | 0.12       |
| (3,1252) | 1:28:A:THR:HG21 | 1:67:A:THR:HG22 | 2                   | 0.12     | 0.02                | 0.12       |
| (3,1252) | 1:28:A:THR:HG21 | 1:67:A:THR:HG23 | 2                   | 0.12     | 0.02                | 0.12       |
| (3,1252) | 1:28:A:THR:HG22 | 1:67:A:THR:HG21 | 2                   | 0.12     | 0.02                | 0.12       |
| (3,1252) | 1:28:A:THR:HG22 | 1:67:A:THR:HG22 | 2                   | 0.12     | 0.02                | 0.12       |
| (3,1252) | 1:28:A:THR:HG22 | 1:67:A:THR:HG23 | 2                   | 0.12     | 0.02                | 0.12       |
| (3,1252) | 1:28:A:THR:HG23 | 1:67:A:THR:HG21 | 2                   | 0.12     | 0.02                | 0.12       |
| (3,1252) | 1:28:A:THR:HG23 | 1:67:A:THR:HG22 | 2                   | 0.12     | 0.02                | 0.12       |
| (3,1252) | 1:28:A:THR:HG23 | 1:67:A:THR:HG23 | 2                   | 0.12     | 0.02                | 0.12       |
| (3,1866) | 1:7:A:ALA:HB1   | 1:8:A:GLU:H     | 2                   | 0.12     | 0.02                | 0.12       |
| (3,1866) | 1:7:A:ALA:HB2   | 1:8:A:GLU:H     | 2                   | 0.12     | 0.02                | 0.12       |

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| Key      | Atom-1          | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (3,1866) | 1:7:A:ALA:HB3   | 1:8:A:GLU:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1623) | 1:82:A:ILE:HG21 | 1:84:A:ARG:HG2 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1623) | 1:82:A:ILE:HG22 | 1:84:A:ARG:HG2 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1623) | 1:82:A:ILE:HG23 | 1:84:A:ARG:HG2 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,3104) | 1:79:A:TYR:HE1  | 1:66:A:MET:HE1 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,3104) | 1:79:A:TYR:HE1  | 1:66:A:MET:HE2 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,3104) | 1:79:A:TYR:HE1  | 1:66:A:MET:HE3 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,3104) | 1:79:A:TYR:HE2  | 1:66:A:MET:HE1 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,3104) | 1:79:A:TYR:HE2  | 1:66:A:MET:HE2 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,3104) | 1:79:A:TYR:HE2  | 1:66:A:MET:HE3 | 2                   | 0.12     | 0.0                 | 0.12       |
| (3,1627) | 1:82:A:ILE:HG21 | 1:84:A:ARG:HG2 | 2                   | 0.12     | 0.01                | 0.12       |
| (3,1627) | 1:82:A:ILE:HG22 | 1:84:A:ARG:HG2 | 2                   | 0.12     | 0.01                | 0.12       |
| (3,1627) | 1:82:A:ILE:HG23 | 1:84:A:ARG:HG2 | 2                   | 0.12     | 0.01                | 0.12       |
| (3,3110) | 1:79:A:TYR:HE1  | 1:66:A:MET:HE1 | 2                   | 0.12     | 0.0                 | 0.12       |
| (3,3110) | 1:79:A:TYR:HE1  | 1:66:A:MET:HE2 | 2                   | 0.12     | 0.0                 | 0.12       |
| (3,3110) | 1:79:A:TYR:HE1  | 1:66:A:MET:HE3 | 2                   | 0.12     | 0.0                 | 0.12       |
| (3,3110) | 1:79:A:TYR:HE2  | 1:66:A:MET:HE1 | 2                   | 0.12     | 0.0                 | 0.12       |
| (3,3110) | 1:79:A:TYR:HE2  | 1:66:A:MET:HE2 | 2                   | 0.12     | 0.0                 | 0.12       |
| (3,3110) | 1:79:A:TYR:HE2  | 1:66:A:MET:HE3 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1725) | 1:38:A:ALA:HB1  | 1:83:A:ALA:HA  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1725) | 1:38:A:ALA:HB2  | 1:83:A:ALA:HA  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1725) | 1:38:A:ALA:HB3  | 1:83:A:ALA:HA  | 2                   | 0.12     | 0.02                | 0.12       |
| (3,1728) | 1:38:A:ALA:HB1  | 1:83:A:ALA:HA  | 2                   | 0.12     | 0.02                | 0.12       |
| (3,1728) | 1:38:A:ALA:HB2  | 1:83:A:ALA:HA  | 2                   | 0.12     | 0.02                | 0.12       |
| (3,1728) | 1:38:A:ALA:HB3  | 1:83:A:ALA:HA  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1037) | 1:56:A:ASN:HD22 | 1:56:A:ASN:HA  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,2054) | 1:78:A:VAL:HG11 | 1:96:A:GLU:HG2 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,2054) | 1:78:A:VAL:HG12 | 1:96:A:GLU:HG2 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,2054) | 1:78:A:VAL:HG13 | 1:96:A:GLU:HG2 | 2                   | 0.12     | 0.0                 | 0.12       |
| (3,1036) | 1:56:A:ASN:HD22 | 1:56:A:ASN:HA  | 2                   | 0.12     | 0.0                 | 0.12       |
| (3,2059) | 1:78:A:VAL:HG11 | 1:96:A:GLU:HG2 | 2                   | 0.12     | 0.0                 | 0.12       |
| (3,2059) | 1:78:A:VAL:HG12 | 1:96:A:GLU:HG2 | 2                   | 0.12     | 0.0                 | 0.12       |
| (3,2059) | 1:78:A:VAL:HG13 | 1:96:A:GLU:HG2 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,24)   | 1:89:A:GLY:H    | 1:9:A:PRO:HB3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,813)  | 1:25:A:GLN:H    | 1:25:A:GLN:HG3 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1130) | 1:40:A:VAL:H    | 1:83:A:ALA:HB1 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1130) | 1:40:A:VAL:H    | 1:83:A:ALA:HB2 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1130) | 1:40:A:VAL:H    | 1:83:A:ALA:HB3 | 2                   | 0.11     | 0.0                 | 0.11       |
| (3,24)   | 1:89:A:GLY:H    | 1:9:A:PRO:HB3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (3,813)  | 1:25:A:GLN:H    | 1:25:A:GLN:HG3 | 2                   | 0.11     | 0.0                 | 0.11       |
| (3,1131) | 1:40:A:VAL:H    | 1:83:A:ALA:HB1 | 2                   | 0.11     | 0.0                 | 0.11       |
| (3,1131) | 1:40:A:VAL:H    | 1:83:A:ALA:HB2 | 2                   | 0.11     | 0.0                 | 0.11       |

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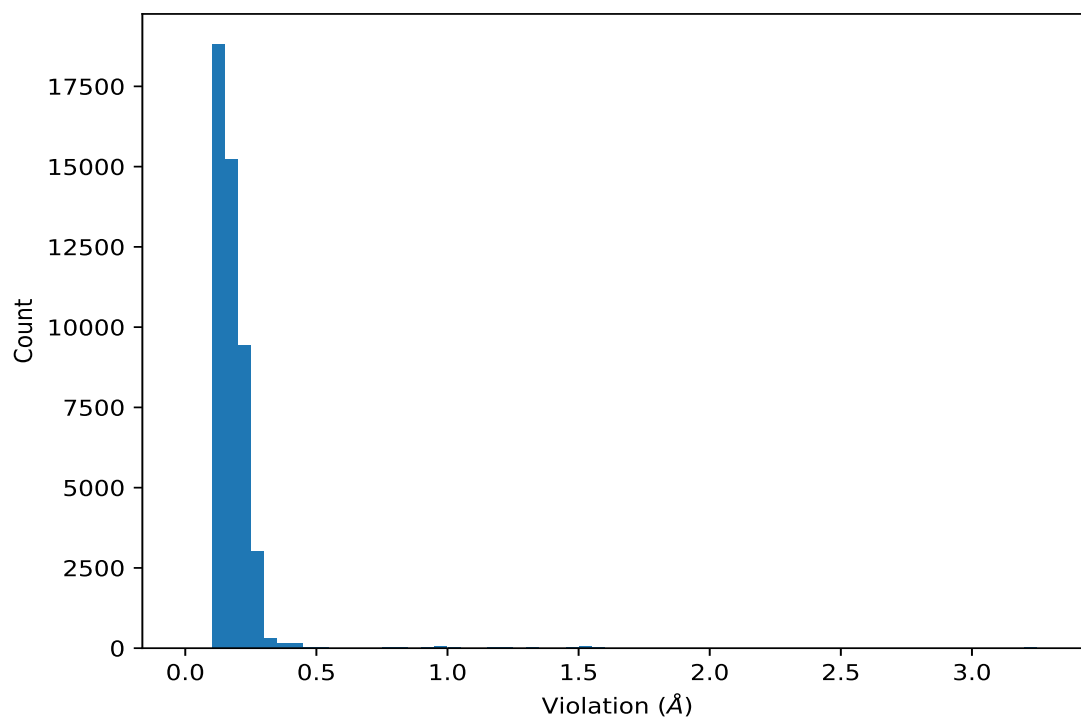
| Key      | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (3,1131) | 1:40:A:VAL:H   | 1:83:A:ALA:HB3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,3183) | 1:43:A:TYR:HE1 | 1:82:A:ILE:HG13 | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,3183) | 1:43:A:TYR:HE2 | 1:82:A:ILE:HG13 | 2                   | 0.1      | 0.0                 | 0.1        |
| (3,2981) | 1:88:A:ARG:HD2 | 1:35:A:PHE:HD1  | 2                   | 0.1      | 0.0                 | 0.1        |
| (3,2981) | 1:88:A:ARG:HD2 | 1:35:A:PHE:HD2  | 2                   | 0.1      | 0.0                 | 0.1        |
| (3,3189) | 1:43:A:TYR:HE1 | 1:82:A:ILE:HG13 | 2                   | 0.1      | 0.0                 | 0.1        |
| (3,3189) | 1:43:A:TYR:HE2 | 1:82:A:ILE:HG13 | 2                   | 0.1      | 0.0                 | 0.1        |

<sup>1</sup>Number of violated models, <sup>2</sup>Standard deviation

## 9.5 All violated distance restraints [i](#)

### 9.5.1 Histogram : Distribution of distance violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



### 9.5.2 Table : All distance violations [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,34)   | 1:88:A:ARG:H   | 1:86:A:GLU:HA  | 16       | 3.29          |
| (3,34)   | 1:88:A:ARG:H   | 1:86:A:GLU:HA  | 3        | 3.27          |
| (3,34)   | 1:88:A:ARG:H   | 1:86:A:GLU:HA  | 18       | 3.27          |
| (3,34)   | 1:88:A:ARG:H   | 1:86:A:GLU:HA  | 19       | 3.27          |
| (3,34)   | 1:88:A:ARG:H   | 1:86:A:GLU:HA  | 9        | 3.26          |
| (3,34)   | 1:88:A:ARG:H   | 1:86:A:GLU:HA  | 11       | 3.26          |
| (3,34)   | 1:88:A:ARG:H   | 1:86:A:GLU:HA  | 12       | 3.26          |
| (3,34)   | 1:88:A:ARG:H   | 1:86:A:GLU:HA  | 13       | 3.26          |
| (3,34)   | 1:88:A:ARG:H   | 1:86:A:GLU:HA  | 6        | 3.24          |
| (3,34)   | 1:88:A:ARG:H   | 1:86:A:GLU:HA  | 7        | 3.24          |
| (3,34)   | 1:88:A:ARG:H   | 1:86:A:GLU:HA  | 10       | 3.24          |
| (3,34)   | 1:88:A:ARG:H   | 1:86:A:GLU:HA  | 14       | 3.24          |
| (3,34)   | 1:88:A:ARG:H   | 1:86:A:GLU:HA  | 15       | 3.24          |
| (3,34)   | 1:88:A:ARG:H   | 1:86:A:GLU:HA  | 17       | 3.24          |
| (3,34)   | 1:88:A:ARG:H   | 1:86:A:GLU:HA  | 1        | 3.23          |
| (3,34)   | 1:88:A:ARG:H   | 1:86:A:GLU:HA  | 5        | 3.23          |
| (3,34)   | 1:88:A:ARG:H   | 1:86:A:GLU:HA  | 20       | 3.23          |
| (3,34)   | 1:88:A:ARG:H   | 1:86:A:GLU:HA  | 4        | 3.22          |
| (3,34)   | 1:88:A:ARG:H   | 1:86:A:GLU:HA  | 8        | 3.22          |
| (3,34)   | 1:88:A:ARG:H   | 1:86:A:GLU:HA  | 2        | 3.2           |
| (3,2749) | 1:86:A:GLU:HG2 | 1:87:A:PRO:HA  | 2        | 3.07          |
| (3,2749) | 1:86:A:GLU:HG2 | 1:87:A:PRO:HA  | 20       | 3.06          |
| (3,32)   | 1:88:A:ARG:H   | 1:86:A:GLU:HG2 | 20       | 2.89          |
| (3,32)   | 1:88:A:ARG:H   | 1:86:A:GLU:HG2 | 2        | 2.84          |
| (3,2748) | 1:86:A:GLU:HG3 | 1:87:A:PRO:HA  | 9        | 2.67          |
| (3,2749) | 1:86:A:GLU:HG2 | 1:87:A:PRO:HA  | 9        | 2.58          |
| (3,32)   | 1:88:A:ARG:H   | 1:86:A:GLU:HG2 | 9        | 2.44          |
| (3,32)   | 1:88:A:ARG:H   | 1:86:A:GLU:HG2 | 6        | 2.43          |
| (3,32)   | 1:88:A:ARG:H   | 1:86:A:GLU:HG2 | 11       | 2.43          |
| (3,32)   | 1:88:A:ARG:H   | 1:86:A:GLU:HG2 | 16       | 2.43          |
| (3,32)   | 1:88:A:ARG:H   | 1:86:A:GLU:HG2 | 13       | 2.42          |
| (3,32)   | 1:88:A:ARG:H   | 1:86:A:GLU:HG2 | 18       | 2.42          |
| (3,32)   | 1:88:A:ARG:H   | 1:86:A:GLU:HG2 | 7        | 2.4           |
| (3,32)   | 1:88:A:ARG:H   | 1:86:A:GLU:HG2 | 10       | 2.38          |
| (3,32)   | 1:88:A:ARG:H   | 1:86:A:GLU:HG2 | 4        | 2.37          |
| (3,32)   | 1:88:A:ARG:H   | 1:86:A:GLU:HG2 | 14       | 2.36          |
| (3,32)   | 1:88:A:ARG:H   | 1:86:A:GLU:HG2 | 1        | 2.35          |
| (3,32)   | 1:88:A:ARG:H   | 1:86:A:GLU:HG2 | 5        | 2.33          |
| (3,32)   | 1:88:A:ARG:H   | 1:86:A:GLU:HG2 | 8        | 2.32          |
| (3,2748) | 1:86:A:GLU:HG3 | 1:87:A:PRO:HA  | 7        | 2.31          |
| (3,2748) | 1:86:A:GLU:HG3 | 1:87:A:PRO:HA  | 10       | 2.3           |
| (3,2748) | 1:86:A:GLU:HG3 | 1:87:A:PRO:HA  | 6        | 2.29          |
| (3,2748) | 1:86:A:GLU:HG3 | 1:87:A:PRO:HA  | 13       | 2.29          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2748) | 1:86:A:GLU:HG3  | 1:87:A:PRO:HA  | 1        | 2.27          |
| (3,2749) | 1:86:A:GLU:HG2  | 1:87:A:PRO:HA  | 13       | 2.26          |
| (3,2749) | 1:86:A:GLU:HG2  | 1:87:A:PRO:HA  | 1        | 2.25          |
| (3,2748) | 1:86:A:GLU:HG3  | 1:87:A:PRO:HA  | 5        | 2.25          |
| (3,2748) | 1:86:A:GLU:HG3  | 1:87:A:PRO:HA  | 8        | 2.25          |
| (3,2748) | 1:86:A:GLU:HG3  | 1:87:A:PRO:HA  | 16       | 2.25          |
| (3,2749) | 1:86:A:GLU:HG2  | 1:87:A:PRO:HA  | 6        | 2.24          |
| (3,2748) | 1:86:A:GLU:HG3  | 1:87:A:PRO:HA  | 18       | 2.24          |
| (3,2749) | 1:86:A:GLU:HG2  | 1:87:A:PRO:HA  | 18       | 2.23          |
| (3,2748) | 1:86:A:GLU:HG3  | 1:87:A:PRO:HA  | 4        | 2.23          |
| (3,2748) | 1:86:A:GLU:HG3  | 1:87:A:PRO:HA  | 11       | 2.23          |
| (3,2748) | 1:86:A:GLU:HG3  | 1:87:A:PRO:HA  | 14       | 2.22          |
| (3,2749) | 1:86:A:GLU:HG2  | 1:87:A:PRO:HA  | 4        | 2.21          |
| (3,2749) | 1:86:A:GLU:HG2  | 1:87:A:PRO:HA  | 11       | 2.21          |
| (3,2749) | 1:86:A:GLU:HG2  | 1:87:A:PRO:HA  | 5        | 2.2           |
| (3,2749) | 1:86:A:GLU:HG2  | 1:87:A:PRO:HA  | 8        | 2.18          |
| (3,2749) | 1:86:A:GLU:HG2  | 1:87:A:PRO:HA  | 10       | 2.17          |
| (3,2749) | 1:86:A:GLU:HG2  | 1:87:A:PRO:HA  | 14       | 2.17          |
| (3,2749) | 1:86:A:GLU:HG2  | 1:87:A:PRO:HA  | 16       | 2.17          |
| (3,2749) | 1:86:A:GLU:HG2  | 1:87:A:PRO:HA  | 7        | 2.16          |
| (3,2748) | 1:86:A:GLU:HG3  | 1:87:A:PRO:HA  | 2        | 2.07          |
| (3,2748) | 1:86:A:GLU:HG3  | 1:87:A:PRO:HA  | 20       | 2.03          |
| (3,2749) | 1:86:A:GLU:HG2  | 1:87:A:PRO:HA  | 12       | 1.87          |
| (3,2749) | 1:86:A:GLU:HG2  | 1:87:A:PRO:HA  | 17       | 1.82          |
| (3,2749) | 1:86:A:GLU:HG2  | 1:87:A:PRO:HA  | 19       | 1.77          |
| (3,2749) | 1:86:A:GLU:HG2  | 1:87:A:PRO:HA  | 3        | 1.76          |
| (3,2749) | 1:86:A:GLU:HG2  | 1:87:A:PRO:HA  | 15       | 1.74          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB2 | 3        | 1.64          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB3 | 3        | 1.64          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB2 | 12       | 1.63          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB3 | 12       | 1.63          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB2 | 19       | 1.62          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB3 | 19       | 1.62          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 29       | 1.61          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 29       | 1.61          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 29       | 1.61          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 19       | 1.59          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 19       | 1.59          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 19       | 1.59          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 33       | 1.57          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 33       | 1.57          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 33       | 1.57          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 1        | 1.56          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 1        | 1.56          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 1        | 1.56          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 16       | 1.56          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 16       | 1.56          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 16       | 1.56          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 17       | 1.56          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 17       | 1.56          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 17       | 1.56          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 23       | 1.56          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 23       | 1.56          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 23       | 1.56          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 3        | 1.55          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 3        | 1.55          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 3        | 1.55          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 6        | 1.55          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 6        | 1.55          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 6        | 1.55          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 12       | 1.55          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 12       | 1.55          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 12       | 1.55          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 37       | 1.55          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 37       | 1.55          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 37       | 1.55          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 2        | 1.54          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 2        | 1.54          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 2        | 1.54          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 35       | 1.54          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 35       | 1.54          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 35       | 1.54          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB2 | 15       | 1.54          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB3 | 15       | 1.54          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 5        | 1.53          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 5        | 1.53          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 5        | 1.53          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 9        | 1.53          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 9        | 1.53          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 9        | 1.53          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 22       | 1.53          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 22       | 1.53          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 22       | 1.53          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 26       | 1.53          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 26       | 1.53          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 26       | 1.53          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 31       | 1.53          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 31       | 1.53          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 31       | 1.53          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 36       | 1.53          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 36       | 1.53          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 36       | 1.53          |
| (3,2753) | 1:86:A:GLU:HB2  | 1:87:A:PRO:HA  | 12       | 1.52          |
| (3,2753) | 1:86:A:GLU:HB3  | 1:87:A:PRO:HA  | 12       | 1.52          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 7        | 1.52          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 7        | 1.52          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 7        | 1.52          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 10       | 1.52          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 10       | 1.52          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 10       | 1.52          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 14       | 1.52          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 14       | 1.52          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 14       | 1.52          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 15       | 1.52          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 15       | 1.52          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 15       | 1.52          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 20       | 1.52          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 20       | 1.52          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 20       | 1.52          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 28       | 1.52          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 28       | 1.52          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 28       | 1.52          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 11       | 1.51          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 11       | 1.51          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 11       | 1.51          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 13       | 1.51          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 13       | 1.51          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 13       | 1.51          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 27       | 1.51          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 27       | 1.51          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 27       | 1.51          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 40       | 1.51          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 40       | 1.51          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 40       | 1.51          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB2 | 17       | 1.51          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB3 | 17       | 1.51          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 4        | 1.5           |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 4        | 1.5           |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 4        | 1.5           |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 8        | 1.5           |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 8        | 1.5           |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 8        | 1.5           |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 18       | 1.5           |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 18       | 1.5           |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 18       | 1.5           |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 30       | 1.5           |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 30       | 1.5           |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 30       | 1.5           |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 25       | 1.49          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 25       | 1.49          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 25       | 1.49          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 34       | 1.49          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 34       | 1.49          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 34       | 1.49          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 39       | 1.49          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 39       | 1.49          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 39       | 1.49          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 38       | 1.48          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 38       | 1.48          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 38       | 1.48          |
| (3,2753) | 1:86:A:GLU:HB2  | 1:87:A:PRO:HA  | 3        | 1.47          |
| (3,2753) | 1:86:A:GLU:HB3  | 1:87:A:PRO:HA  | 3        | 1.47          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 32       | 1.47          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 32       | 1.47          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 32       | 1.47          |
| (3,2753) | 1:86:A:GLU:HB2  | 1:87:A:PRO:HA  | 15       | 1.46          |
| (3,2753) | 1:86:A:GLU:HB3  | 1:87:A:PRO:HA  | 15       | 1.46          |
| (3,2753) | 1:86:A:GLU:HB2  | 1:87:A:PRO:HA  | 17       | 1.46          |
| (3,2753) | 1:86:A:GLU:HB3  | 1:87:A:PRO:HA  | 17       | 1.46          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 21       | 1.46          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 21       | 1.46          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 21       | 1.46          |
| (3,1673) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 24       | 1.46          |
| (3,1673) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 24       | 1.46          |
| (3,1673) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 24       | 1.46          |
| (3,2753) | 1:86:A:GLU:HB2  | 1:87:A:PRO:HA  | 19       | 1.45          |
| (3,2753) | 1:86:A:GLU:HB3  | 1:87:A:PRO:HA  | 19       | 1.45          |
| (3,2529) | 1:87:A:PRO:HB3  | 1:86:A:GLU:HA  | 13       | 1.45          |

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| Key      | Atom-1         | Atom-2        | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (3,2529) | 1:87:A:PRO:HB3 | 1:86:A:GLU:HA | 6        | 1.44          |
| (3,2529) | 1:87:A:PRO:HB3 | 1:86:A:GLU:HA | 9        | 1.44          |
| (3,2529) | 1:87:A:PRO:HB3 | 1:86:A:GLU:HA | 10       | 1.44          |
| (3,2529) | 1:87:A:PRO:HB3 | 1:86:A:GLU:HA | 12       | 1.44          |
| (3,2529) | 1:87:A:PRO:HB3 | 1:86:A:GLU:HA | 7        | 1.43          |
| (3,2529) | 1:87:A:PRO:HB3 | 1:86:A:GLU:HA | 1        | 1.39          |
| (3,2529) | 1:87:A:PRO:HB3 | 1:86:A:GLU:HA | 18       | 1.39          |
| (3,2529) | 1:87:A:PRO:HB3 | 1:86:A:GLU:HA | 2        | 1.37          |
| (3,2529) | 1:87:A:PRO:HB3 | 1:86:A:GLU:HA | 5        | 1.37          |
| (3,2529) | 1:87:A:PRO:HB3 | 1:86:A:GLU:HA | 15       | 1.36          |
| (3,2529) | 1:87:A:PRO:HB3 | 1:86:A:GLU:HA | 16       | 1.36          |
| (3,2529) | 1:87:A:PRO:HB3 | 1:86:A:GLU:HA | 4        | 1.34          |
| (3,2529) | 1:87:A:PRO:HB3 | 1:86:A:GLU:HA | 8        | 1.34          |
| (3,2529) | 1:87:A:PRO:HB3 | 1:86:A:GLU:HA | 11       | 1.34          |
| (3,2529) | 1:87:A:PRO:HB3 | 1:86:A:GLU:HA | 20       | 1.34          |
| (3,2529) | 1:87:A:PRO:HB3 | 1:86:A:GLU:HA | 3        | 1.33          |
| (3,2529) | 1:87:A:PRO:HB3 | 1:86:A:GLU:HA | 19       | 1.33          |
| (3,2753) | 1:86:A:GLU:HB2 | 1:87:A:PRO:HA | 9        | 1.31          |
| (3,2753) | 1:86:A:GLU:HB3 | 1:87:A:PRO:HA | 9        | 1.31          |
| (3,2529) | 1:87:A:PRO:HB3 | 1:86:A:GLU:HA | 14       | 1.31          |
| (3,2753) | 1:86:A:GLU:HB2 | 1:87:A:PRO:HA | 6        | 1.3           |
| (3,2753) | 1:86:A:GLU:HB3 | 1:87:A:PRO:HA | 6        | 1.3           |
| (3,2753) | 1:86:A:GLU:HB2 | 1:87:A:PRO:HA | 7        | 1.3           |
| (3,2753) | 1:86:A:GLU:HB3 | 1:87:A:PRO:HA | 7        | 1.3           |
| (3,2753) | 1:86:A:GLU:HB2 | 1:87:A:PRO:HA | 13       | 1.29          |
| (3,2753) | 1:86:A:GLU:HB3 | 1:87:A:PRO:HA | 13       | 1.29          |
| (3,2529) | 1:87:A:PRO:HB3 | 1:86:A:GLU:HA | 17       | 1.29          |
| (3,2753) | 1:86:A:GLU:HB2 | 1:87:A:PRO:HA | 10       | 1.27          |
| (3,2753) | 1:86:A:GLU:HB3 | 1:87:A:PRO:HA | 10       | 1.27          |
| (3,2753) | 1:86:A:GLU:HB2 | 1:87:A:PRO:HA | 1        | 1.24          |
| (3,2753) | 1:86:A:GLU:HB3 | 1:87:A:PRO:HA | 1        | 1.24          |
| (3,2753) | 1:86:A:GLU:HB2 | 1:87:A:PRO:HA | 11       | 1.24          |
| (3,2753) | 1:86:A:GLU:HB3 | 1:87:A:PRO:HA | 11       | 1.24          |
| (3,2753) | 1:86:A:GLU:HB2 | 1:87:A:PRO:HA | 16       | 1.24          |
| (3,2753) | 1:86:A:GLU:HB3 | 1:87:A:PRO:HA | 16       | 1.24          |
| (3,2753) | 1:86:A:GLU:HB2 | 1:87:A:PRO:HA | 14       | 1.23          |
| (3,2753) | 1:86:A:GLU:HB3 | 1:87:A:PRO:HA | 14       | 1.23          |
| (3,2753) | 1:86:A:GLU:HB2 | 1:87:A:PRO:HA | 8        | 1.22          |
| (3,2753) | 1:86:A:GLU:HB3 | 1:87:A:PRO:HA | 8        | 1.22          |
| (3,2753) | 1:86:A:GLU:HB2 | 1:87:A:PRO:HA | 4        | 1.21          |
| (3,2753) | 1:86:A:GLU:HB3 | 1:87:A:PRO:HA | 4        | 1.21          |
| (3,2753) | 1:86:A:GLU:HB2 | 1:87:A:PRO:HA | 5        | 1.21          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2753) | 1:86:A:GLU:HB3  | 1:87:A:PRO:HA  | 5        | 1.21          |
| (3,2753) | 1:86:A:GLU:HB2  | 1:87:A:PRO:HA  | 18       | 1.21          |
| (3,2753) | 1:86:A:GLU:HB3  | 1:87:A:PRO:HA  | 18       | 1.21          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB2 | 7        | 1.21          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB3 | 7        | 1.21          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB2 | 9        | 1.19          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB3 | 9        | 1.19          |
| (3,2753) | 1:86:A:GLU:HB2  | 1:87:A:PRO:HA  | 2        | 1.18          |
| (3,2753) | 1:86:A:GLU:HB3  | 1:87:A:PRO:HA  | 2        | 1.18          |
| (3,2753) | 1:86:A:GLU:HB2  | 1:87:A:PRO:HA  | 20       | 1.18          |
| (3,2753) | 1:86:A:GLU:HB3  | 1:87:A:PRO:HA  | 20       | 1.18          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB2 | 6        | 1.16          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB3 | 6        | 1.16          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB2 | 10       | 1.16          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB3 | 10       | 1.16          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB2 | 16       | 1.16          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB3 | 16       | 1.16          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB2 | 11       | 1.13          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB3 | 11       | 1.13          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB2 | 13       | 1.13          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB3 | 13       | 1.13          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB2 | 20       | 1.11          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB3 | 20       | 1.11          |
| (3,22)   | 1:89:A:GLY:H    | 1:85:A:LEU:H   | 5        | 1.11          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB2 | 18       | 1.09          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB3 | 18       | 1.09          |
| (3,22)   | 1:89:A:GLY:H    | 1:85:A:LEU:H   | 4        | 1.07          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB2 | 2        | 1.06          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB3 | 2        | 1.06          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB2 | 14       | 1.06          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB3 | 14       | 1.06          |
| (3,22)   | 1:89:A:GLY:H    | 1:85:A:LEU:H   | 1        | 1.06          |
| (3,22)   | 1:89:A:GLY:H    | 1:85:A:LEU:H   | 8        | 1.05          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB2 | 4        | 1.04          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB3 | 4        | 1.04          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB2 | 8        | 1.01          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB3 | 8        | 1.01          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 27       | 1.0           |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 27       | 1.0           |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 27       | 1.0           |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 29       | 1.0           |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 29       | 1.0           |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 29       | 1.0           |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB2 | 1        | 1.0           |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB3 | 1        | 1.0           |
| (3,22)   | 1:89:A:GLY:H    | 1:85:A:LEU:H   | 9        | 0.99          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 22       | 0.98          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 22       | 0.98          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 22       | 0.98          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 23       | 0.98          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 23       | 0.98          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 23       | 0.98          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 31       | 0.98          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 31       | 0.98          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 31       | 0.98          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 35       | 0.98          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 35       | 0.98          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 35       | 0.98          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB2 | 5        | 0.98          |
| (3,33)   | 1:88:A:ARG:H    | 1:86:A:GLU:HB3 | 5        | 0.98          |
| (3,22)   | 1:89:A:GLY:H    | 1:85:A:LEU:H   | 6        | 0.98          |
| (3,22)   | 1:89:A:GLY:H    | 1:85:A:LEU:H   | 20       | 0.98          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 25       | 0.97          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 25       | 0.97          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 25       | 0.97          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 33       | 0.97          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 33       | 0.97          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 33       | 0.97          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 39       | 0.97          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 39       | 0.97          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 39       | 0.97          |
| (3,32)   | 1:88:A:ARG:H    | 1:86:A:GLU:HG2 | 12       | 0.97          |
| (3,22)   | 1:89:A:GLY:H    | 1:85:A:LEU:H   | 3        | 0.97          |
| (3,22)   | 1:89:A:GLY:H    | 1:85:A:LEU:H   | 12       | 0.97          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 26       | 0.96          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 26       | 0.96          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 26       | 0.96          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 28       | 0.96          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 28       | 0.96          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 28       | 0.96          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 36       | 0.96          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 36       | 0.96          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 36       | 0.96          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 37       | 0.96          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 37       | 0.96          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 37       | 0.96          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 40       | 0.96          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 40       | 0.96          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 40       | 0.96          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 24       | 0.95          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 24       | 0.95          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 24       | 0.95          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 32       | 0.95          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 32       | 0.95          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 32       | 0.95          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 38       | 0.95          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 38       | 0.95          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 38       | 0.95          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 21       | 0.94          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 21       | 0.94          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 21       | 0.94          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 30       | 0.94          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 30       | 0.94          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 30       | 0.94          |
| (3,32)   | 1:88:A:ARG:H    | 1:86:A:GLU:HG2 | 3        | 0.94          |
| (3,32)   | 1:88:A:ARG:H    | 1:86:A:GLU:HG2 | 19       | 0.94          |
| (3,22)   | 1:89:A:GLY:H    | 1:85:A:LEU:H   | 10       | 0.94          |
| (3,22)   | 1:89:A:GLY:H    | 1:85:A:LEU:H   | 16       | 0.94          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 34       | 0.93          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 34       | 0.93          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 34       | 0.93          |
| (3,1149) | 1:86:A:GLU:H    | 1:87:A:PRO:HA  | 6        | 0.93          |
| (3,22)   | 1:89:A:GLY:H    | 1:85:A:LEU:H   | 7        | 0.93          |
| (3,1149) | 1:86:A:GLU:H    | 1:87:A:PRO:HA  | 7        | 0.92          |
| (3,1149) | 1:86:A:GLU:H    | 1:87:A:PRO:HA  | 9        | 0.91          |
| (3,1149) | 1:86:A:GLU:H    | 1:87:A:PRO:HA  | 10       | 0.91          |
| (3,22)   | 1:89:A:GLY:H    | 1:85:A:LEU:H   | 15       | 0.91          |
| (3,22)   | 1:89:A:GLY:H    | 1:85:A:LEU:H   | 18       | 0.91          |
| (3,1149) | 1:86:A:GLU:H    | 1:87:A:PRO:HA  | 12       | 0.9           |
| (3,1149) | 1:86:A:GLU:H    | 1:87:A:PRO:HA  | 13       | 0.89          |
| (3,32)   | 1:88:A:ARG:H    | 1:86:A:GLU:HG2 | 17       | 0.88          |
| (3,22)   | 1:89:A:GLY:H    | 1:85:A:LEU:H   | 14       | 0.87          |
| (3,1149) | 1:86:A:GLU:H    | 1:87:A:PRO:HA  | 2        | 0.86          |
| (3,22)   | 1:89:A:GLY:H    | 1:85:A:LEU:H   | 2        | 0.86          |
| (3,22)   | 1:89:A:GLY:H    | 1:85:A:LEU:H   | 11       | 0.85          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 2        | 0.84          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 2        | 0.84          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 2        | 0.84          |
| (3,1149) | 1:86:A:GLU:H    | 1:87:A:PRO:HA  | 1        | 0.84          |
| (3,22)   | 1:89:A:GLY:H    | 1:85:A:LEU:H   | 19       | 0.84          |
| (3,2749) | 1:86:A:GLU:HG2  | 1:87:A:PRO:HA  | 27       | 0.83          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 13       | 0.83          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 13       | 0.83          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 13       | 0.83          |
| (3,1149) | 1:86:A:GLU:H    | 1:87:A:PRO:HA  | 20       | 0.83          |
| (3,22)   | 1:89:A:GLY:H    | 1:85:A:LEU:H   | 17       | 0.83          |
| (3,1149) | 1:86:A:GLU:H    | 1:87:A:PRO:HA  | 15       | 0.82          |
| (3,1149) | 1:86:A:GLU:H    | 1:87:A:PRO:HA  | 18       | 0.82          |
| (3,32)   | 1:88:A:ARG:H    | 1:86:A:GLU:HG2 | 15       | 0.82          |
| (3,1149) | 1:86:A:GLU:H    | 1:87:A:PRO:HA  | 14       | 0.81          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 1        | 0.8           |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 1        | 0.8           |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 1        | 0.8           |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 5        | 0.8           |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 5        | 0.8           |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 5        | 0.8           |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 6        | 0.8           |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 6        | 0.8           |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 6        | 0.8           |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 11       | 0.8           |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 11       | 0.8           |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 11       | 0.8           |
| (3,1149) | 1:86:A:GLU:H    | 1:87:A:PRO:HA  | 5        | 0.8           |
| (3,1149) | 1:86:A:GLU:H    | 1:87:A:PRO:HA  | 8        | 0.8           |
| (3,1149) | 1:86:A:GLU:H    | 1:87:A:PRO:HA  | 16       | 0.8           |
| (3,1149) | 1:86:A:GLU:H    | 1:87:A:PRO:HA  | 19       | 0.8           |
| (3,22)   | 1:89:A:GLY:H    | 1:85:A:LEU:H   | 13       | 0.8           |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 16       | 0.79          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 16       | 0.79          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 16       | 0.79          |
| (3,1149) | 1:86:A:GLU:H    | 1:87:A:PRO:HA  | 3        | 0.79          |
| (3,1149) | 1:86:A:GLU:H    | 1:87:A:PRO:HA  | 4        | 0.79          |
| (3,1149) | 1:86:A:GLU:H    | 1:87:A:PRO:HA  | 17       | 0.79          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 4        | 0.78          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 4        | 0.78          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 4        | 0.78          |
| (3,1149) | 1:86:A:GLU:H    | 1:87:A:PRO:HA  | 11       | 0.78          |
| (3,32)   | 1:88:A:ARG:H    | 1:86:A:GLU:HG2 | 28       | 0.78          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 10       | 0.77          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 10       | 0.77          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 10       | 0.77          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 14       | 0.77          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 14       | 0.77          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 14       | 0.77          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 19       | 0.77          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 19       | 0.77          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 19       | 0.77          |
| (3,32)   | 1:88:A:ARG:H    | 1:86:A:GLU:HG2 | 29       | 0.77          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 12       | 0.76          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 12       | 0.76          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 12       | 0.76          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 15       | 0.76          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 15       | 0.76          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 15       | 0.76          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 17       | 0.76          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 17       | 0.76          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 17       | 0.76          |
| (3,32)   | 1:88:A:ARG:H    | 1:86:A:GLU:HG2 | 35       | 0.76          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 3        | 0.75          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 3        | 0.75          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 3        | 0.75          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 8        | 0.75          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 8        | 0.75          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 8        | 0.75          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 9        | 0.75          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 9        | 0.75          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 9        | 0.75          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 20       | 0.74          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 20       | 0.74          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 20       | 0.74          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 7        | 0.73          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 7        | 0.73          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 7        | 0.73          |
| (3,2069) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 18       | 0.73          |
| (3,2069) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 18       | 0.73          |
| (3,2069) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 18       | 0.73          |
| (3,32)   | 1:88:A:ARG:H    | 1:86:A:GLU:HG2 | 27       | 0.72          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2 | 11       | 0.68          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 6        | 0.57          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 7        | 0.57          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 12       | 0.57          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 13       | 0.57          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 9        | 0.56          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 10       | 0.55          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 17       | 0.55          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 1        | 0.54          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 3        | 0.54          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 5        | 0.54          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 8        | 0.54          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 11       | 0.54          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 14       | 0.54          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 16       | 0.54          |
| (3,2749) | 1:86:A:GLU:HG2  | 1:87:A:PRO:HA  | 28       | 0.53          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 15       | 0.53          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 19       | 0.53          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 20       | 0.53          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 2        | 0.52          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 4        | 0.52          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 18       | 0.52          |
| (3,2749) | 1:86:A:GLU:HG2  | 1:87:A:PRO:HA  | 29       | 0.51          |
| (3,2749) | 1:86:A:GLU:HG2  | 1:87:A:PRO:HA  | 35       | 0.51          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 25       | 0.51          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 27       | 0.51          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 39       | 0.5           |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 29       | 0.49          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 38       | 0.49          |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 28       | 0.48          |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 28       | 0.48          |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 28       | 0.48          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 22       | 0.48          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 23       | 0.48          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 24       | 0.48          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 28       | 0.48          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 32       | 0.48          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 34       | 0.48          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 35       | 0.48          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 21       | 0.47          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 30       | 0.47          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 31       | 0.47          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 33       | 0.47          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 36       | 0.47          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 37       | 0.47          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 40       | 0.47          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 2        | 0.46          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 9        | 0.46          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 11       | 0.46          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 15       | 0.46          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 18       | 0.46          |
| (3,1241) | 1:13:A:THR:HG21 | 1:34:A:SER:HB2 | 6        | 0.46          |
| (3,1241) | 1:13:A:THR:HG22 | 1:34:A:SER:HB2 | 6        | 0.46          |
| (3,1241) | 1:13:A:THR:HG23 | 1:34:A:SER:HB2 | 6        | 0.46          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 10       | 0.45          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 12       | 0.45          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 13       | 0.45          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 16       | 0.45          |
| (3,37)   | 1:88:A:ARG:H    | 1:88:A:ARG:HG2 | 26       | 0.45          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 1        | 0.44          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 4        | 0.44          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 6        | 0.44          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 7        | 0.44          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 14       | 0.44          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 17       | 0.44          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 20       | 0.44          |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 8        | 0.44          |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 8        | 0.44          |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 8        | 0.44          |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 16       | 0.44          |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 16       | 0.44          |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 16       | 0.44          |
| (3,1241) | 1:13:A:THR:HG21 | 1:34:A:SER:HB2 | 26       | 0.44          |
| (3,1241) | 1:13:A:THR:HG22 | 1:34:A:SER:HB2 | 26       | 0.44          |
| (3,1241) | 1:13:A:THR:HG23 | 1:34:A:SER:HB2 | 26       | 0.44          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 3        | 0.43          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 5        | 0.43          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 8        | 0.43          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 19       | 0.43          |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 12       | 0.43          |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 12       | 0.43          |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 12       | 0.43          |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 29       | 0.43          |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 29       | 0.43          |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 29       | 0.43          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2 | 6        | 0.43          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2 | 17       | 0.43          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 3        | 0.42          |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 3        | 0.42          |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 3        | 0.42          |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 4        | 0.42          |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 4        | 0.42          |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 4        | 0.42          |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 10       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 10       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 10       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 19       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 19       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 19       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 20       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 20       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 20       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 24       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 24       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 24       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 30       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 30       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 30       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 31       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 31       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 31       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 33       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 33       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 33       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 35       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 35       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 35       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 36       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 36       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 36       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 37       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 37       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 37       | 0.42          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2 | 2        | 0.42          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2 | 27       | 0.42          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2 | 28       | 0.42          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2 | 37       | 0.42          |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 2        | 0.41          |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 2        | 0.41          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 2        | 0.41          |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 5        | 0.41          |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 5        | 0.41          |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 5        | 0.41          |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 6        | 0.41          |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 6        | 0.41          |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 6        | 0.41          |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 9        | 0.41          |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 9        | 0.41          |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 9        | 0.41          |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 11       | 0.41          |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 11       | 0.41          |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 11       | 0.41          |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 22       | 0.41          |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 22       | 0.41          |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 22       | 0.41          |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 23       | 0.41          |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 23       | 0.41          |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 23       | 0.41          |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 25       | 0.41          |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 25       | 0.41          |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 25       | 0.41          |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 32       | 0.41          |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 32       | 0.41          |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 32       | 0.41          |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 39       | 0.41          |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 39       | 0.41          |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 39       | 0.41          |
| (3,1241) | 1:13:A:THR:HG21 | 1:34:A:SER:HB2 | 9        | 0.41          |
| (3,1241) | 1:13:A:THR:HG22 | 1:34:A:SER:HB2 | 9        | 0.41          |
| (3,1241) | 1:13:A:THR:HG23 | 1:34:A:SER:HB2 | 9        | 0.41          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2 | 1        | 0.41          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2 | 21       | 0.41          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2 | 30       | 0.41          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2 | 34       | 0.41          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 29       | 0.41          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 29       | 0.41          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 29       | 0.41          |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 1        | 0.4           |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 1        | 0.4           |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 1        | 0.4           |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 7        | 0.4           |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 7        | 0.4           |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 7        | 0.4           |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 13       | 0.4           |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 13       | 0.4           |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 13       | 0.4           |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 15       | 0.4           |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 15       | 0.4           |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 15       | 0.4           |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 17       | 0.4           |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 17       | 0.4           |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 17       | 0.4           |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 18       | 0.4           |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 18       | 0.4           |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 18       | 0.4           |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 21       | 0.4           |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 21       | 0.4           |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 21       | 0.4           |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 26       | 0.4           |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 26       | 0.4           |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 26       | 0.4           |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 34       | 0.4           |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 34       | 0.4           |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 34       | 0.4           |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 38       | 0.4           |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 38       | 0.4           |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 38       | 0.4           |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 40       | 0.4           |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 40       | 0.4           |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 40       | 0.4           |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2 | 4        | 0.4           |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2 | 23       | 0.4           |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2 | 24       | 0.4           |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2 | 25       | 0.4           |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2 | 26       | 0.4           |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2 | 35       | 0.4           |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2 | 36       | 0.4           |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 27       | 0.4           |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 27       | 0.4           |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 27       | 0.4           |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 29       | 0.4           |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 29       | 0.4           |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 29       | 0.4           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H    | 27       | 0.39          |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H    | 27       | 0.39          |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H    | 27       | 0.39          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2  | 7        | 0.39          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2  | 8        | 0.39          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2  | 16       | 0.39          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2  | 20       | 0.39          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2  | 22       | 0.39          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2  | 33       | 0.39          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2  | 40       | 0.39          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3  | 19       | 0.39          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3  | 19       | 0.39          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3  | 19       | 0.39          |
| (3,3218) | 1:65:A:TYR:HE1  | 1:58:A:ARG:HB3  | 6        | 0.38          |
| (3,3218) | 1:65:A:TYR:HE2  | 1:58:A:ARG:HB3  | 6        | 0.38          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3   | 33       | 0.38          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2  | 9        | 0.38          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2  | 12       | 0.38          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2  | 13       | 0.38          |
| (1,3212) | 1:65:A:TYR:HE1  | 1:58:A:ARG:HB3  | 6        | 0.38          |
| (1,3212) | 1:65:A:TYR:HE2  | 1:58:A:ARG:HB3  | 6        | 0.38          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3  | 22       | 0.38          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3  | 22       | 0.38          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3  | 22       | 0.38          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3  | 23       | 0.38          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3  | 23       | 0.38          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3  | 23       | 0.38          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3  | 31       | 0.38          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3  | 31       | 0.38          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3  | 31       | 0.38          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3  | 35       | 0.38          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3  | 35       | 0.38          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3  | 35       | 0.38          |
| (3,2601) | 1:36:A:ASP:HB3  | 1:37:A:ASP:H    | 1        | 0.37          |
| (3,2601) | 1:36:A:ASP:HB3  | 1:37:A:ASP:H    | 18       | 0.37          |
| (3,2318) | 1:80:A:SER:HA   | 1:94:A:THR:HG21 | 28       | 0.37          |
| (3,2318) | 1:80:A:SER:HA   | 1:94:A:THR:HG22 | 28       | 0.37          |
| (3,2318) | 1:80:A:SER:HA   | 1:94:A:THR:HG23 | 28       | 0.37          |
| (3,1353) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H    | 14       | 0.37          |
| (3,1353) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H    | 14       | 0.37          |
| (3,1353) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H    | 14       | 0.37          |
| (3,919)  | 1:37:A:ASP:H    | 1:36:A:ASP:HB3  | 1        | 0.37          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,919)  | 1:37:A:ASP:H    | 1:36:A:ASP:HB3  | 18       | 0.37          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2  | 10       | 0.37          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2  | 31       | 0.37          |
| (3,546)  | 1:71:A:VAL:H    | 1:24:A:HIS:HA   | 18       | 0.37          |
| (3,176)  | 1:10:A:ILE:H    | 1:35:A:PHE:HD1  | 11       | 0.37          |
| (3,176)  | 1:10:A:ILE:H    | 1:35:A:PHE:HD2  | 11       | 0.37          |
| (1,2597) | 1:36:A:ASP:HB3  | 1:37:A:ASP:H    | 1        | 0.37          |
| (1,2597) | 1:36:A:ASP:HB3  | 1:37:A:ASP:H    | 18       | 0.37          |
| (1,2315) | 1:80:A:SER:HA   | 1:94:A:THR:HG21 | 28       | 0.37          |
| (1,2315) | 1:80:A:SER:HA   | 1:94:A:THR:HG22 | 28       | 0.37          |
| (1,2315) | 1:80:A:SER:HA   | 1:94:A:THR:HG23 | 28       | 0.37          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3  | 25       | 0.37          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3  | 25       | 0.37          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3  | 25       | 0.37          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3  | 33       | 0.37          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3  | 33       | 0.37          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3  | 33       | 0.37          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3  | 39       | 0.37          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3  | 39       | 0.37          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3  | 39       | 0.37          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3  | 33       | 0.37          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3  | 33       | 0.37          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3  | 33       | 0.37          |
| (1,918)  | 1:37:A:ASP:H    | 1:36:A:ASP:HB3  | 1        | 0.37          |
| (1,918)  | 1:37:A:ASP:H    | 1:36:A:ASP:HB3  | 18       | 0.37          |
| (1,546)  | 1:71:A:VAL:H    | 1:24:A:HIS:HA   | 18       | 0.37          |
| (1,176)  | 1:10:A:ILE:H    | 1:35:A:PHE:HD1  | 11       | 0.37          |
| (1,176)  | 1:10:A:ILE:H    | 1:35:A:PHE:HD2  | 11       | 0.37          |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG21 | 5        | 0.36          |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG22 | 5        | 0.36          |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG23 | 5        | 0.36          |
| (3,2601) | 1:36:A:ASP:HB3  | 1:37:A:ASP:H    | 40       | 0.36          |
| (3,2485) | 1:9:A:PRO:HD3   | 1:9:A:PRO:HB3   | 2        | 0.36          |
| (3,2485) | 1:9:A:PRO:HD3   | 1:9:A:PRO:HB3   | 9        | 0.36          |
| (3,2485) | 1:9:A:PRO:HD3   | 1:9:A:PRO:HB3   | 11       | 0.36          |
| (3,2485) | 1:9:A:PRO:HD3   | 1:9:A:PRO:HB3   | 15       | 0.36          |
| (3,2485) | 1:9:A:PRO:HD3   | 1:9:A:PRO:HB3   | 18       | 0.36          |
| (3,919)  | 1:37:A:ASP:H    | 1:36:A:ASP:HB3  | 40       | 0.36          |
| (3,862)  | 1:86:A:GLU:H    | 1:85:A:LEU:H    | 3        | 0.36          |
| (3,862)  | 1:86:A:GLU:H    | 1:85:A:LEU:H    | 7        | 0.36          |
| (3,862)  | 1:86:A:GLU:H    | 1:85:A:LEU:H    | 9        | 0.36          |
| (3,862)  | 1:86:A:GLU:H    | 1:85:A:LEU:H    | 12       | 0.36          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2  | 3        | 0.36          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2  | 5        | 0.36          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2  | 29       | 0.36          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2  | 32       | 0.36          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2  | 38       | 0.36          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2  | 39       | 0.36          |
| (3,546)  | 1:71:A:VAL:H    | 1:24:A:HIS:HA   | 17       | 0.36          |
| (1,3004) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG21 | 5        | 0.36          |
| (1,3004) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG22 | 5        | 0.36          |
| (1,3004) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG23 | 5        | 0.36          |
| (1,2597) | 1:36:A:ASP:HB3  | 1:37:A:ASP:H    | 40       | 0.36          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3  | 26       | 0.36          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3  | 26       | 0.36          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3  | 26       | 0.36          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3  | 28       | 0.36          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3  | 28       | 0.36          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3  | 28       | 0.36          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3  | 36       | 0.36          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3  | 36       | 0.36          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3  | 36       | 0.36          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3  | 37       | 0.36          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3  | 37       | 0.36          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3  | 37       | 0.36          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3  | 40       | 0.36          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3  | 40       | 0.36          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3  | 40       | 0.36          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3  | 1        | 0.36          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3  | 1        | 0.36          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3  | 1        | 0.36          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3  | 16       | 0.36          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3  | 16       | 0.36          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3  | 16       | 0.36          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3  | 17       | 0.36          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3  | 17       | 0.36          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3  | 17       | 0.36          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3  | 23       | 0.36          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3  | 23       | 0.36          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3  | 23       | 0.36          |
| (1,918)  | 1:37:A:ASP:H    | 1:36:A:ASP:HB3  | 40       | 0.36          |
| (1,546)  | 1:71:A:VAL:H    | 1:24:A:HIS:HA   | 17       | 0.36          |
| (3,3133) | 1:55:A:TYR:HD1  | 1:49:A:LEU:HB2  | 15       | 0.35          |
| (3,3133) | 1:55:A:TYR:HD2  | 1:49:A:LEU:HB2  | 15       | 0.35          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 26       | 0.35          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 27       | 0.35          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 29       | 0.35          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 37       | 0.35          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 40       | 0.35          |
| (3,2485) | 1:9:A:PRO:HD3   | 1:9:A:PRO:HB3  | 10       | 0.35          |
| (3,2485) | 1:9:A:PRO:HD3   | 1:9:A:PRO:HB3  | 12       | 0.35          |
| (3,2485) | 1:9:A:PRO:HD3   | 1:9:A:PRO:HB3  | 13       | 0.35          |
| (3,2485) | 1:9:A:PRO:HD3   | 1:9:A:PRO:HB3  | 16       | 0.35          |
| (3,862)  | 1:86:A:GLU:H    | 1:85:A:LEU:H   | 6        | 0.35          |
| (3,862)  | 1:86:A:GLU:H    | 1:85:A:LEU:H   | 10       | 0.35          |
| (3,862)  | 1:86:A:GLU:H    | 1:85:A:LEU:H   | 13       | 0.35          |
| (3,862)  | 1:86:A:GLU:H    | 1:85:A:LEU:H   | 16       | 0.35          |
| (3,862)  | 1:86:A:GLU:H    | 1:85:A:LEU:H   | 17       | 0.35          |
| (3,862)  | 1:86:A:GLU:H    | 1:85:A:LEU:H   | 19       | 0.35          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2 | 14       | 0.35          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2 | 15       | 0.35          |
| (1,3127) | 1:55:A:TYR:HD1  | 1:49:A:LEU:HB2 | 15       | 0.35          |
| (1,3127) | 1:55:A:TYR:HD2  | 1:49:A:LEU:HB2 | 15       | 0.35          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 24       | 0.35          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 24       | 0.35          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 24       | 0.35          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 32       | 0.35          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 32       | 0.35          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 32       | 0.35          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 38       | 0.35          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 38       | 0.35          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 38       | 0.35          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 3        | 0.35          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 3        | 0.35          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 3        | 0.35          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 6        | 0.35          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 6        | 0.35          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 6        | 0.35          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 12       | 0.35          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 12       | 0.35          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 12       | 0.35          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 37       | 0.35          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 37       | 0.35          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 37       | 0.35          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 28       | 0.34          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 30       | 0.34          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 31       | 0.34          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 34       | 0.34          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 38       | 0.34          |
| (3,2485) | 1:9:A:PRO:HD3   | 1:9:A:PRO:HB3  | 1        | 0.34          |
| (3,2485) | 1:9:A:PRO:HD3   | 1:9:A:PRO:HB3  | 4        | 0.34          |
| (3,2485) | 1:9:A:PRO:HD3   | 1:9:A:PRO:HB3  | 6        | 0.34          |
| (3,2485) | 1:9:A:PRO:HD3   | 1:9:A:PRO:HB3  | 7        | 0.34          |
| (3,2485) | 1:9:A:PRO:HD3   | 1:9:A:PRO:HB3  | 14       | 0.34          |
| (3,2485) | 1:9:A:PRO:HD3   | 1:9:A:PRO:HB3  | 17       | 0.34          |
| (3,2485) | 1:9:A:PRO:HD3   | 1:9:A:PRO:HB3  | 20       | 0.34          |
| (3,862)  | 1:86:A:GLU:H    | 1:85:A:LEU:H   | 2        | 0.34          |
| (3,862)  | 1:86:A:GLU:H    | 1:85:A:LEU:H   | 8        | 0.34          |
| (3,862)  | 1:86:A:GLU:H    | 1:85:A:LEU:H   | 11       | 0.34          |
| (3,862)  | 1:86:A:GLU:H    | 1:85:A:LEU:H   | 14       | 0.34          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 21       | 0.34          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 21       | 0.34          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 21       | 0.34          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 30       | 0.34          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 30       | 0.34          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 30       | 0.34          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 2        | 0.34          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 2        | 0.34          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 2        | 0.34          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 35       | 0.34          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 35       | 0.34          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 35       | 0.34          |
| (3,3218) | 1:65:A:TYR:HE1  | 1:58:A:ARG:HB3 | 2        | 0.33          |
| (3,3218) | 1:65:A:TYR:HE2  | 1:58:A:ARG:HB3 | 2        | 0.33          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 21       | 0.33          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 24       | 0.33          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 25       | 0.33          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 36       | 0.33          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 39       | 0.33          |
| (3,2601) | 1:36:A:ASP:HB3  | 1:37:A:ASP:H   | 29       | 0.33          |
| (3,2485) | 1:9:A:PRO:HD3   | 1:9:A:PRO:HB3  | 3        | 0.33          |
| (3,2485) | 1:9:A:PRO:HD3   | 1:9:A:PRO:HB3  | 5        | 0.33          |
| (3,2485) | 1:9:A:PRO:HD3   | 1:9:A:PRO:HB3  | 8        | 0.33          |
| (3,2485) | 1:9:A:PRO:HD3   | 1:9:A:PRO:HB3  | 19       | 0.33          |
| (3,919)  | 1:37:A:ASP:H    | 1:36:A:ASP:HB3 | 29       | 0.33          |
| (3,862)  | 1:86:A:GLU:H    | 1:85:A:LEU:H   | 1        | 0.33          |
| (3,862)  | 1:86:A:GLU:H    | 1:85:A:LEU:H   | 4        | 0.33          |
| (3,862)  | 1:86:A:GLU:H    | 1:85:A:LEU:H   | 5        | 0.33          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,862)  | 1:86:A:GLU:H    | 1:85:A:LEU:H   | 15       | 0.33          |
| (3,862)  | 1:86:A:GLU:H    | 1:85:A:LEU:H   | 18       | 0.33          |
| (3,862)  | 1:86:A:GLU:H    | 1:85:A:LEU:H   | 20       | 0.33          |
| (3,584)  | 1:93:A:SER:H    | 1:92:A:ARG:HB2 | 18       | 0.33          |
| (3,563)  | 1:47:A:THR:H    | 1:45:A:GLY:HA2 | 18       | 0.33          |
| (3,176)  | 1:10:A:ILE:H    | 1:35:A:PHE:HD1 | 3        | 0.33          |
| (3,176)  | 1:10:A:ILE:H    | 1:35:A:PHE:HD2 | 3        | 0.33          |
| (3,125)  | 1:55:A:TYR:H    | 1:54:A:LYS:H   | 32       | 0.33          |
| (1,3212) | 1:65:A:TYR:HE1  | 1:58:A:ARG:HB3 | 2        | 0.33          |
| (1,3212) | 1:65:A:TYR:HE2  | 1:58:A:ARG:HB3 | 2        | 0.33          |
| (1,2597) | 1:36:A:ASP:HB3  | 1:37:A:ASP:H   | 29       | 0.33          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 34       | 0.33          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 34       | 0.33          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 34       | 0.33          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 5        | 0.33          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 5        | 0.33          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 5        | 0.33          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 9        | 0.33          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 9        | 0.33          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 9        | 0.33          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 22       | 0.33          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 22       | 0.33          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 22       | 0.33          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 26       | 0.33          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 26       | 0.33          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 26       | 0.33          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 31       | 0.33          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 31       | 0.33          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 31       | 0.33          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 36       | 0.33          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 36       | 0.33          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 36       | 0.33          |
| (1,918)  | 1:37:A:ASP:H    | 1:36:A:ASP:HB3 | 29       | 0.33          |
| (1,584)  | 1:93:A:SER:H    | 1:92:A:ARG:HB2 | 18       | 0.33          |
| (1,176)  | 1:10:A:ILE:H    | 1:35:A:PHE:HD1 | 3        | 0.33          |
| (1,176)  | 1:10:A:ILE:H    | 1:35:A:PHE:HD2 | 3        | 0.33          |
| (1,149)  | 1:45:A:GLY:H    | 1:46:A:PRO:HD3 | 14       | 0.33          |
| (1,149)  | 1:45:A:GLY:H    | 1:46:A:PRO:HD3 | 16       | 0.33          |
| (1,123)  | 1:55:A:TYR:H    | 1:54:A:LYS:H   | 32       | 0.33          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 22       | 0.32          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 32       | 0.32          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 35       | 0.32          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 31       | 0.32          |
| (3,546)  | 1:71:A:VAL:H    | 1:24:A:HIS:HA  | 29       | 0.32          |
| (3,125)  | 1:55:A:TYR:H    | 1:54:A:LYS:H   | 16       | 0.32          |
| (3,125)  | 1:55:A:TYR:H    | 1:54:A:LYS:H   | 36       | 0.32          |
| (3,125)  | 1:55:A:TYR:H    | 1:54:A:LYS:H   | 38       | 0.32          |
| (3,22)   | 1:89:A:GLY:H    | 1:85:A:LEU:H   | 33       | 0.32          |
| (1,2511) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 31       | 0.32          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 7        | 0.32          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 7        | 0.32          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 7        | 0.32          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 10       | 0.32          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 10       | 0.32          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 10       | 0.32          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 14       | 0.32          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 14       | 0.32          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 14       | 0.32          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 15       | 0.32          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 15       | 0.32          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 15       | 0.32          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 20       | 0.32          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 20       | 0.32          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 20       | 0.32          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 28       | 0.32          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 28       | 0.32          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 28       | 0.32          |
| (1,546)  | 1:71:A:VAL:H    | 1:24:A:HIS:HA  | 29       | 0.32          |
| (1,123)  | 1:55:A:TYR:H    | 1:54:A:LYS:H   | 16       | 0.32          |
| (1,123)  | 1:55:A:TYR:H    | 1:54:A:LYS:H   | 36       | 0.32          |
| (1,123)  | 1:55:A:TYR:H    | 1:54:A:LYS:H   | 38       | 0.32          |
| (3,3218) | 1:65:A:TYR:HE1  | 1:58:A:ARG:HB3 | 12       | 0.31          |
| (3,3218) | 1:65:A:TYR:HE2  | 1:58:A:ARG:HB3 | 12       | 0.31          |
| (3,2925) | 1:22:A:SER:HB2  | 1:25:A:GLN:H   | 28       | 0.31          |
| (3,2925) | 1:22:A:SER:HB2  | 1:25:A:GLN:H   | 29       | 0.31          |
| (3,2925) | 1:22:A:SER:HB2  | 1:25:A:GLN:H   | 31       | 0.31          |
| (3,2649) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 23       | 0.31          |
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 21       | 0.31          |
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 22       | 0.31          |
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 23       | 0.31          |
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 24       | 0.31          |
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 25       | 0.31          |
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 27       | 0.31          |
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 34       | 0.31          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 36       | 0.31          |
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 37       | 0.31          |
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 39       | 0.31          |
| (3,584)  | 1:93:A:SER:H    | 1:92:A:ARG:HB2 | 1        | 0.31          |
| (3,176)  | 1:10:A:ILE:H    | 1:35:A:PHE:HD1 | 6        | 0.31          |
| (3,176)  | 1:10:A:ILE:H    | 1:35:A:PHE:HD2 | 6        | 0.31          |
| (3,176)  | 1:10:A:ILE:H    | 1:35:A:PHE:HD1 | 10       | 0.31          |
| (3,176)  | 1:10:A:ILE:H    | 1:35:A:PHE:HD2 | 10       | 0.31          |
| (3,176)  | 1:10:A:ILE:H    | 1:35:A:PHE:HD1 | 18       | 0.31          |
| (3,176)  | 1:10:A:ILE:H    | 1:35:A:PHE:HD2 | 18       | 0.31          |
| (3,125)  | 1:55:A:TYR:H    | 1:54:A:LYS:H   | 1        | 0.31          |
| (3,125)  | 1:55:A:TYR:H    | 1:54:A:LYS:H   | 3        | 0.31          |
| (3,125)  | 1:55:A:TYR:H    | 1:54:A:LYS:H   | 12       | 0.31          |
| (3,125)  | 1:55:A:TYR:H    | 1:54:A:LYS:H   | 14       | 0.31          |
| (3,125)  | 1:55:A:TYR:H    | 1:54:A:LYS:H   | 18       | 0.31          |
| (3,125)  | 1:55:A:TYR:H    | 1:54:A:LYS:H   | 19       | 0.31          |
| (3,125)  | 1:55:A:TYR:H    | 1:54:A:LYS:H   | 22       | 0.31          |
| (3,125)  | 1:55:A:TYR:H    | 1:54:A:LYS:H   | 25       | 0.31          |
| (3,125)  | 1:55:A:TYR:H    | 1:54:A:LYS:H   | 26       | 0.31          |
| (3,125)  | 1:55:A:TYR:H    | 1:54:A:LYS:H   | 28       | 0.31          |
| (3,125)  | 1:55:A:TYR:H    | 1:54:A:LYS:H   | 34       | 0.31          |
| (3,125)  | 1:55:A:TYR:H    | 1:54:A:LYS:H   | 35       | 0.31          |
| (1,3212) | 1:65:A:TYR:HE1  | 1:58:A:ARG:HB3 | 12       | 0.31          |
| (1,3212) | 1:65:A:TYR:HE2  | 1:58:A:ARG:HB3 | 12       | 0.31          |
| (1,2918) | 1:22:A:SER:HB2  | 1:25:A:GLN:H   | 28       | 0.31          |
| (1,2918) | 1:22:A:SER:HB2  | 1:25:A:GLN:H   | 29       | 0.31          |
| (1,2918) | 1:22:A:SER:HB2  | 1:25:A:GLN:H   | 31       | 0.31          |
| (1,2511) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 21       | 0.31          |
| (1,2511) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 22       | 0.31          |
| (1,2511) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 23       | 0.31          |
| (1,2511) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 24       | 0.31          |
| (1,2511) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 25       | 0.31          |
| (1,2511) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 27       | 0.31          |
| (1,2511) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 34       | 0.31          |
| (1,2511) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 36       | 0.31          |
| (1,2511) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 37       | 0.31          |
| (1,2511) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 39       | 0.31          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 11       | 0.31          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 11       | 0.31          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3 | 11       | 0.31          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3 | 13       | 0.31          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3 | 13       | 0.31          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3  | 13       | 0.31          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3  | 27       | 0.31          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3  | 27       | 0.31          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3  | 27       | 0.31          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3  | 40       | 0.31          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3  | 40       | 0.31          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3  | 40       | 0.31          |
| (1,584)  | 1:93:A:SER:H    | 1:92:A:ARG:HB2  | 1        | 0.31          |
| (1,199)  | 1:90:A:GLU:H    | 1:10:A:ILE:HG21 | 26       | 0.31          |
| (1,199)  | 1:90:A:GLU:H    | 1:10:A:ILE:HG22 | 26       | 0.31          |
| (1,199)  | 1:90:A:GLU:H    | 1:10:A:ILE:HG23 | 26       | 0.31          |
| (1,176)  | 1:10:A:ILE:H    | 1:35:A:PHE:HD1  | 6        | 0.31          |
| (1,176)  | 1:10:A:ILE:H    | 1:35:A:PHE:HD2  | 6        | 0.31          |
| (1,176)  | 1:10:A:ILE:H    | 1:35:A:PHE:HD1  | 10       | 0.31          |
| (1,176)  | 1:10:A:ILE:H    | 1:35:A:PHE:HD2  | 10       | 0.31          |
| (1,176)  | 1:10:A:ILE:H    | 1:35:A:PHE:HD1  | 18       | 0.31          |
| (1,176)  | 1:10:A:ILE:H    | 1:35:A:PHE:HD2  | 18       | 0.31          |
| (1,149)  | 1:45:A:GLY:H    | 1:46:A:PRO:HD3  | 2        | 0.31          |
| (1,149)  | 1:45:A:GLY:H    | 1:46:A:PRO:HD3  | 5        | 0.31          |
| (1,149)  | 1:45:A:GLY:H    | 1:46:A:PRO:HD3  | 18       | 0.31          |
| (1,123)  | 1:55:A:TYR:H    | 1:54:A:LYS:H    | 1        | 0.31          |
| (1,123)  | 1:55:A:TYR:H    | 1:54:A:LYS:H    | 3        | 0.31          |
| (1,123)  | 1:55:A:TYR:H    | 1:54:A:LYS:H    | 12       | 0.31          |
| (1,123)  | 1:55:A:TYR:H    | 1:54:A:LYS:H    | 14       | 0.31          |
| (1,123)  | 1:55:A:TYR:H    | 1:54:A:LYS:H    | 18       | 0.31          |
| (1,123)  | 1:55:A:TYR:H    | 1:54:A:LYS:H    | 19       | 0.31          |
| (1,123)  | 1:55:A:TYR:H    | 1:54:A:LYS:H    | 22       | 0.31          |
| (1,123)  | 1:55:A:TYR:H    | 1:54:A:LYS:H    | 25       | 0.31          |
| (1,123)  | 1:55:A:TYR:H    | 1:54:A:LYS:H    | 26       | 0.31          |
| (1,123)  | 1:55:A:TYR:H    | 1:54:A:LYS:H    | 28       | 0.31          |
| (1,123)  | 1:55:A:TYR:H    | 1:54:A:LYS:H    | 34       | 0.31          |
| (1,123)  | 1:55:A:TYR:H    | 1:54:A:LYS:H    | 35       | 0.31          |
| (3,3056) | 1:60:A:ASP:HB2  | 1:63:A:CYS:HB2  | 4        | 0.3           |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG21 | 9        | 0.3           |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG22 | 9        | 0.3           |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG23 | 9        | 0.3           |
| (3,2925) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 13       | 0.3           |
| (3,2925) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 36       | 0.3           |
| (3,2684) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HG3  | 35       | 0.3           |
| (3,2676) | 1:25:A:GLN:HG3  | 1:22:A:SER:HB2  | 6        | 0.3           |
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2  | 26       | 0.3           |
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2  | 28       | 0.3           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2  | 29       | 0.3           |
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2  | 30       | 0.3           |
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2  | 33       | 0.3           |
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2  | 35       | 0.3           |
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2  | 38       | 0.3           |
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2  | 40       | 0.3           |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 3        | 0.3           |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 3        | 0.3           |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 3        | 0.3           |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 6        | 0.3           |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 6        | 0.3           |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 6        | 0.3           |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 37       | 0.3           |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 37       | 0.3           |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 37       | 0.3           |
| (3,1188) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 3        | 0.3           |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 3        | 0.3           |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 3        | 0.3           |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD23 | 3        | 0.3           |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 6        | 0.3           |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 6        | 0.3           |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD23 | 6        | 0.3           |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 37       | 0.3           |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 37       | 0.3           |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD23 | 37       | 0.3           |
| (3,584)  | 1:93:A:SER:H    | 1:92:A:ARG:HB2  | 27       | 0.3           |
| (3,176)  | 1:10:A:ILE:H    | 1:35:A:PHE:HD1  | 1        | 0.3           |
| (3,176)  | 1:10:A:ILE:H    | 1:35:A:PHE:HD2  | 1        | 0.3           |
| (3,176)  | 1:10:A:ILE:H    | 1:35:A:PHE:HD1  | 7        | 0.3           |
| (3,176)  | 1:10:A:ILE:H    | 1:35:A:PHE:HD2  | 7        | 0.3           |
| (3,125)  | 1:55:A:TYR:H    | 1:54:A:LYS:H    | 2        | 0.3           |
| (3,125)  | 1:55:A:TYR:H    | 1:54:A:LYS:H    | 8        | 0.3           |
| (3,125)  | 1:55:A:TYR:H    | 1:54:A:LYS:H    | 9        | 0.3           |
| (3,125)  | 1:55:A:TYR:H    | 1:54:A:LYS:H    | 21       | 0.3           |
| (3,125)  | 1:55:A:TYR:H    | 1:54:A:LYS:H    | 23       | 0.3           |
| (3,125)  | 1:55:A:TYR:H    | 1:54:A:LYS:H    | 31       | 0.3           |
| (3,125)  | 1:55:A:TYR:H    | 1:54:A:LYS:H    | 37       | 0.3           |
| (1,3048) | 1:60:A:ASP:HB2  | 1:63:A:CYS:HB2  | 4        | 0.3           |
| (1,3004) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG21 | 9        | 0.3           |
| (1,3004) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG22 | 9        | 0.3           |
| (1,3004) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG23 | 9        | 0.3           |
| (1,2918) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 13       | 0.3           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2918) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 36       | 0.3           |
| (1,2680) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HG3  | 35       | 0.3           |
| (1,2672) | 1:25:A:GLN:HG3  | 1:22:A:SER:HB2  | 6        | 0.3           |
| (1,2511) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2  | 26       | 0.3           |
| (1,2511) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2  | 28       | 0.3           |
| (1,2511) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2  | 29       | 0.3           |
| (1,2511) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2  | 30       | 0.3           |
| (1,2511) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2  | 33       | 0.3           |
| (1,2511) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2  | 35       | 0.3           |
| (1,2511) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2  | 38       | 0.3           |
| (1,2511) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2  | 40       | 0.3           |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 3        | 0.3           |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 3        | 0.3           |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 3        | 0.3           |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 6        | 0.3           |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 6        | 0.3           |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 6        | 0.3           |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 37       | 0.3           |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 37       | 0.3           |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 37       | 0.3           |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3  | 4        | 0.3           |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3  | 4        | 0.3           |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3  | 4        | 0.3           |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3  | 8        | 0.3           |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3  | 8        | 0.3           |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3  | 8        | 0.3           |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3  | 18       | 0.3           |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3  | 18       | 0.3           |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3  | 18       | 0.3           |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3  | 30       | 0.3           |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3  | 30       | 0.3           |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3  | 30       | 0.3           |
| (1,1184) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 3        | 0.3           |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 3        | 0.3           |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 3        | 0.3           |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD23 | 3        | 0.3           |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 6        | 0.3           |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 6        | 0.3           |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD23 | 6        | 0.3           |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 37       | 0.3           |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 37       | 0.3           |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD23 | 37       | 0.3           |

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| Key      | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|----------|---------------|----------------|----------|---------------|
| (1,584)  | 1:93:A:SER:H  | 1:92:A:ARG:HB2 | 27       | 0.3           |
| (1,176)  | 1:10:A:ILE:H  | 1:35:A:PHE:HD1 | 1        | 0.3           |
| (1,176)  | 1:10:A:ILE:H  | 1:35:A:PHE:HD2 | 1        | 0.3           |
| (1,176)  | 1:10:A:ILE:H  | 1:35:A:PHE:HD1 | 7        | 0.3           |
| (1,176)  | 1:10:A:ILE:H  | 1:35:A:PHE:HD2 | 7        | 0.3           |
| (1,149)  | 1:45:A:GLY:H  | 1:46:A:PRO:HD3 | 8        | 0.3           |
| (1,123)  | 1:55:A:TYR:H  | 1:54:A:LYS:H   | 2        | 0.3           |
| (1,123)  | 1:55:A:TYR:H  | 1:54:A:LYS:H   | 8        | 0.3           |
| (1,123)  | 1:55:A:TYR:H  | 1:54:A:LYS:H   | 9        | 0.3           |
| (1,123)  | 1:55:A:TYR:H  | 1:54:A:LYS:H   | 21       | 0.3           |
| (1,123)  | 1:55:A:TYR:H  | 1:54:A:LYS:H   | 23       | 0.3           |
| (1,123)  | 1:55:A:TYR:H  | 1:54:A:LYS:H   | 31       | 0.3           |
| (1,123)  | 1:55:A:TYR:H  | 1:54:A:LYS:H   | 37       | 0.3           |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1  | 2        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2  | 2        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1  | 2        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2  | 2        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1  | 3        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2  | 3        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1  | 3        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2  | 3        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1  | 4        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2  | 4        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1  | 4        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2  | 4        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1  | 5        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2  | 5        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1  | 5        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2  | 5        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1  | 6        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2  | 6        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1  | 6        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2  | 6        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1  | 7        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2  | 7        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1  | 7        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2  | 7        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1  | 8        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2  | 8        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1  | 8        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2  | 8        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1  | 9        | 0.29          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 9        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 9        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 9        | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 10       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 10       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 10       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 10       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 11       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 11       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 11       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 11       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 12       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 12       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 12       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 12       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 13       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 13       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 13       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 13       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 14       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 14       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 14       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 14       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 15       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 15       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 15       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 15       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 16       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 16       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 16       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 16       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 17       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 17       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 17       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 17       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 18       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 18       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 18       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 18       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 19       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 19       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 19       | 0.29          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 19       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 20       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 20       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 20       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 20       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 21       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 21       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 21       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 21       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 22       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 22       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 22       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 22       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 24       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 24       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 24       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 24       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 25       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 25       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 25       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 25       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 26       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 26       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 26       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 26       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 27       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 27       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 27       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 27       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 28       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 28       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 28       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 28       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 29       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 29       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 29       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 29       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 30       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 30       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 30       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 30       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 31       | 0.29          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,3176) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE2  | 31       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE1  | 31       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE2  | 31       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE1  | 32       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE2  | 32       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE1  | 32       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE2  | 32       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE1  | 33       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE2  | 33       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE1  | 33       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE2  | 33       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE1  | 34       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE2  | 34       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE1  | 34       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE2  | 34       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE1  | 35       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE2  | 35       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE1  | 35       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE2  | 35       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE1  | 36       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE2  | 36       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE1  | 36       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE2  | 36       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE1  | 37       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE2  | 37       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE1  | 37       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE2  | 37       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE1  | 38       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE2  | 38       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE1  | 38       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE2  | 38       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE1  | 39       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE2  | 39       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE1  | 39       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE2  | 39       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3 | 1:11:A:GLN:HB3 | 1        | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3 | 1:11:A:GLN:HB3 | 2        | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3 | 1:11:A:GLN:HB3 | 3        | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3 | 1:11:A:GLN:HB3 | 4        | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3 | 1:11:A:GLN:HB3 | 5        | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3 | 1:11:A:GLN:HB3 | 6        | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3 | 1:11:A:GLN:HB3 | 7        | 0.29          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 8        | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 9        | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 10       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 11       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 12       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 13       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 14       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 15       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 16       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 17       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 19       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 20       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 21       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 22       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 23       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 24       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 25       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 26       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 27       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 28       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 29       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 30       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 31       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 32       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 33       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 34       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 35       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 36       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 37       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 38       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 39       | 0.29          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 40       | 0.29          |
| (3,2925) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 10       | 0.29          |
| (3,2925) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 33       | 0.29          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 13       | 0.29          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 35       | 0.29          |
| (3,2763) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 38       | 0.29          |
| (3,2682) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HA   | 5        | 0.29          |
| (3,2682) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HA   | 8        | 0.29          |
| (3,2682) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HA   | 9        | 0.29          |
| (3,2682) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HA   | 10       | 0.29          |
| (3,2682) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HA   | 11       | 0.29          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2682) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HA  | 15       | 0.29          |
| (3,2682) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HA  | 16       | 0.29          |
| (3,2682) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HA  | 21       | 0.29          |
| (3,2682) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HA  | 23       | 0.29          |
| (3,2682) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HA  | 24       | 0.29          |
| (3,2682) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HA  | 34       | 0.29          |
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 32       | 0.29          |
| (3,2440) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3 | 38       | 0.29          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 7        | 0.29          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 7        | 0.29          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 7        | 0.29          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 8        | 0.29          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 8        | 0.29          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 8        | 0.29          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 11       | 0.29          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 11       | 0.29          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 11       | 0.29          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 12       | 0.29          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 12       | 0.29          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 12       | 0.29          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 14       | 0.29          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 14       | 0.29          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 14       | 0.29          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 26       | 0.29          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 26       | 0.29          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 26       | 0.29          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 29       | 0.29          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 29       | 0.29          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 29       | 0.29          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 32       | 0.29          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 32       | 0.29          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 32       | 0.29          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 34       | 0.29          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 34       | 0.29          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 34       | 0.29          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 40       | 0.29          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 40       | 0.29          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 40       | 0.29          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA  | 19       | 0.29          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA  | 19       | 0.29          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA  | 19       | 0.29          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H   | 17       | 0.29          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H    | 17       | 0.29          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H    | 17       | 0.29          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H    | 18       | 0.29          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H    | 18       | 0.29          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H    | 18       | 0.29          |
| (3,1166) | 1:97:A:LEU:H    | 1:29:A:PHE:HE1  | 5        | 0.29          |
| (3,1166) | 1:97:A:LEU:H    | 1:29:A:PHE:HE2  | 5        | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 7        | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 7        | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD23 | 7        | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 8        | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 8        | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD23 | 8        | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 11       | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 11       | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD23 | 11       | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 12       | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 12       | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD23 | 12       | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 14       | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 14       | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD23 | 14       | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 26       | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 26       | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD23 | 26       | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 29       | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 29       | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD23 | 29       | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 32       | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 32       | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD23 | 32       | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 34       | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 34       | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD23 | 34       | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 40       | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 40       | 0.29          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD23 | 40       | 0.29          |
| (3,584)  | 1:93:A:SER:H    | 1:92:A:ARG:HB2  | 6        | 0.29          |
| (3,584)  | 1:93:A:SER:H    | 1:92:A:ARG:HB2  | 11       | 0.29          |
| (3,584)  | 1:93:A:SER:H    | 1:92:A:ARG:HB2  | 22       | 0.29          |
| (3,584)  | 1:93:A:SER:H    | 1:92:A:ARG:HB2  | 25       | 0.29          |
| (3,584)  | 1:93:A:SER:H    | 1:92:A:ARG:HB2  | 28       | 0.29          |

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| Key      | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|----------|---------------|----------------|----------|---------------|
| (3,584)  | 1:93:A:SER:H  | 1:92:A:ARG:HB2 | 31       | 0.29          |
| (3,584)  | 1:93:A:SER:H  | 1:92:A:ARG:HB2 | 32       | 0.29          |
| (3,563)  | 1:47:A:THR:H  | 1:45:A:GLY:HA2 | 19       | 0.29          |
| (3,546)  | 1:71:A:VAL:H  | 1:24:A:HIS:HA  | 14       | 0.29          |
| (3,176)  | 1:10:A:ILE:H  | 1:35:A:PHE:HD1 | 12       | 0.29          |
| (3,176)  | 1:10:A:ILE:H  | 1:35:A:PHE:HD2 | 12       | 0.29          |
| (3,176)  | 1:10:A:ILE:H  | 1:35:A:PHE:HD1 | 19       | 0.29          |
| (3,176)  | 1:10:A:ILE:H  | 1:35:A:PHE:HD2 | 19       | 0.29          |
| (3,176)  | 1:10:A:ILE:H  | 1:35:A:PHE:HD1 | 21       | 0.29          |
| (3,176)  | 1:10:A:ILE:H  | 1:35:A:PHE:HD2 | 21       | 0.29          |
| (3,125)  | 1:55:A:TYR:H  | 1:54:A:LYS:H   | 6        | 0.29          |
| (3,125)  | 1:55:A:TYR:H  | 1:54:A:LYS:H   | 10       | 0.29          |
| (3,125)  | 1:55:A:TYR:H  | 1:54:A:LYS:H   | 11       | 0.29          |
| (3,125)  | 1:55:A:TYR:H  | 1:54:A:LYS:H   | 13       | 0.29          |
| (3,125)  | 1:55:A:TYR:H  | 1:54:A:LYS:H   | 15       | 0.29          |
| (3,125)  | 1:55:A:TYR:H  | 1:54:A:LYS:H   | 17       | 0.29          |
| (3,125)  | 1:55:A:TYR:H  | 1:54:A:LYS:H   | 20       | 0.29          |
| (3,125)  | 1:55:A:TYR:H  | 1:54:A:LYS:H   | 29       | 0.29          |
| (3,125)  | 1:55:A:TYR:H  | 1:54:A:LYS:H   | 33       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1  | 2        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2  | 2        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1  | 2        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2  | 2        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1  | 3        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2  | 3        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1  | 3        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2  | 3        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1  | 4        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2  | 4        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1  | 4        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2  | 4        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1  | 5        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2  | 5        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1  | 5        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2  | 5        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1  | 6        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2  | 6        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1  | 6        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2  | 6        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1  | 7        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2  | 7        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1  | 7        | 0.29          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 7        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 8        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 8        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 8        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 8        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 9        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 9        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 9        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 9        | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 10       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 10       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 10       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 10       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 11       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 11       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 11       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 11       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 12       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 12       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 12       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 12       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 13       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 13       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 13       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 13       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 14       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 14       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 14       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 14       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 15       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 15       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 15       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 15       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 16       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 16       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 16       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 16       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 17       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 17       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 17       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 17       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 18       | 0.29          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 18       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 18       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 18       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 19       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 19       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 19       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 19       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 20       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 20       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 20       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 20       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 21       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 21       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 21       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 21       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 22       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 22       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 22       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 22       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 24       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 24       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 24       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 24       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 25       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 25       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 25       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 25       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 26       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 26       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 26       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 26       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 27       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 27       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 27       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 27       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 28       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 28       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 28       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2 | 28       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1 | 29       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2 | 29       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1 | 29       | 0.29          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,3170) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE2  | 29       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE1  | 30       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE2  | 30       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE1  | 30       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE2  | 30       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE1  | 31       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE2  | 31       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE1  | 31       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE2  | 31       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE1  | 32       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE2  | 32       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE1  | 32       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE2  | 32       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE1  | 33       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE2  | 33       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE1  | 33       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE2  | 33       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE1  | 34       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE2  | 34       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE1  | 34       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE2  | 34       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE1  | 35       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE2  | 35       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE1  | 35       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE2  | 35       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE1  | 36       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE2  | 36       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE1  | 36       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE2  | 36       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE1  | 37       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE2  | 37       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE1  | 37       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE2  | 37       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE1  | 38       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE2  | 38       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE1  | 38       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE2  | 38       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE1  | 39       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD1  | 1:5:A:PHE:HE2  | 39       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE1  | 39       | 0.29          |
| (1,3170) | 1:5:A:PHE:HD2  | 1:5:A:PHE:HE2  | 39       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3 | 1:11:A:GLN:HB3 | 1        | 0.29          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 2        | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 3        | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 4        | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 5        | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 6        | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 7        | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 8        | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 9        | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 10       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 11       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 12       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 13       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 14       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 15       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 16       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 17       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 19       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 20       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 21       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 22       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 23       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 24       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 25       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 26       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 27       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 28       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 29       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 30       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 31       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 32       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 33       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 34       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 35       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 36       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 37       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 38       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 39       | 0.29          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 40       | 0.29          |
| (1,2918) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 10       | 0.29          |
| (1,2918) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 33       | 0.29          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 13       | 0.29          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 35       | 0.29          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2756) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA  | 38       | 0.29          |
| (1,2678) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HA  | 5        | 0.29          |
| (1,2678) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HA  | 8        | 0.29          |
| (1,2678) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HA  | 9        | 0.29          |
| (1,2678) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HA  | 10       | 0.29          |
| (1,2678) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HA  | 11       | 0.29          |
| (1,2678) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HA  | 15       | 0.29          |
| (1,2678) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HA  | 16       | 0.29          |
| (1,2678) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HA  | 21       | 0.29          |
| (1,2678) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HA  | 23       | 0.29          |
| (1,2678) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HA  | 24       | 0.29          |
| (1,2678) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HA  | 34       | 0.29          |
| (1,2511) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 32       | 0.29          |
| (1,2437) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3 | 38       | 0.29          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 7        | 0.29          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 7        | 0.29          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 7        | 0.29          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 8        | 0.29          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 8        | 0.29          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 8        | 0.29          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 11       | 0.29          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 11       | 0.29          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 11       | 0.29          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 12       | 0.29          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 12       | 0.29          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 12       | 0.29          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 14       | 0.29          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 14       | 0.29          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 14       | 0.29          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 26       | 0.29          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 26       | 0.29          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 26       | 0.29          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 29       | 0.29          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 29       | 0.29          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 29       | 0.29          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 32       | 0.29          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 32       | 0.29          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 32       | 0.29          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 34       | 0.29          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 34       | 0.29          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 34       | 0.29          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 40       | 0.29          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 40       | 0.29          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 40       | 0.29          |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 19       | 0.29          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 19       | 0.29          |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 19       | 0.29          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3  | 25       | 0.29          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3  | 25       | 0.29          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3  | 25       | 0.29          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3  | 34       | 0.29          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3  | 34       | 0.29          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3  | 34       | 0.29          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3  | 39       | 0.29          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3  | 39       | 0.29          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3  | 39       | 0.29          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H    | 17       | 0.29          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H    | 17       | 0.29          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H    | 17       | 0.29          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H    | 18       | 0.29          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H    | 18       | 0.29          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H    | 18       | 0.29          |
| (1,1162) | 1:97:A:LEU:H    | 1:29:A:PHE:HE1  | 5        | 0.29          |
| (1,1162) | 1:97:A:LEU:H    | 1:29:A:PHE:HE2  | 5        | 0.29          |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 7        | 0.29          |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 7        | 0.29          |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD23 | 7        | 0.29          |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 8        | 0.29          |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 8        | 0.29          |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD23 | 8        | 0.29          |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 11       | 0.29          |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 11       | 0.29          |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD23 | 11       | 0.29          |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 12       | 0.29          |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 12       | 0.29          |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD23 | 12       | 0.29          |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 14       | 0.29          |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 14       | 0.29          |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD23 | 14       | 0.29          |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 26       | 0.29          |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 26       | 0.29          |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD23 | 26       | 0.29          |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 29       | 0.29          |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 29       | 0.29          |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,934)  | 1:98:A:LYS:H  | 1:97:A:LEU:HD23 | 29       | 0.29          |
| (1,934)  | 1:98:A:LYS:H  | 1:97:A:LEU:HD21 | 32       | 0.29          |
| (1,934)  | 1:98:A:LYS:H  | 1:97:A:LEU:HD22 | 32       | 0.29          |
| (1,934)  | 1:98:A:LYS:H  | 1:97:A:LEU:HD23 | 32       | 0.29          |
| (1,934)  | 1:98:A:LYS:H  | 1:97:A:LEU:HD21 | 34       | 0.29          |
| (1,934)  | 1:98:A:LYS:H  | 1:97:A:LEU:HD22 | 34       | 0.29          |
| (1,934)  | 1:98:A:LYS:H  | 1:97:A:LEU:HD23 | 34       | 0.29          |
| (1,934)  | 1:98:A:LYS:H  | 1:97:A:LEU:HD21 | 40       | 0.29          |
| (1,934)  | 1:98:A:LYS:H  | 1:97:A:LEU:HD22 | 40       | 0.29          |
| (1,934)  | 1:98:A:LYS:H  | 1:97:A:LEU:HD23 | 40       | 0.29          |
| (1,584)  | 1:93:A:SER:H  | 1:92:A:ARG:HB2  | 6        | 0.29          |
| (1,584)  | 1:93:A:SER:H  | 1:92:A:ARG:HB2  | 11       | 0.29          |
| (1,584)  | 1:93:A:SER:H  | 1:92:A:ARG:HB2  | 22       | 0.29          |
| (1,584)  | 1:93:A:SER:H  | 1:92:A:ARG:HB2  | 25       | 0.29          |
| (1,584)  | 1:93:A:SER:H  | 1:92:A:ARG:HB2  | 28       | 0.29          |
| (1,584)  | 1:93:A:SER:H  | 1:92:A:ARG:HB2  | 31       | 0.29          |
| (1,584)  | 1:93:A:SER:H  | 1:92:A:ARG:HB2  | 32       | 0.29          |
| (1,546)  | 1:71:A:VAL:H  | 1:24:A:HIS:HA   | 14       | 0.29          |
| (1,199)  | 1:90:A:GLU:H  | 1:10:A:ILE:HG21 | 37       | 0.29          |
| (1,199)  | 1:90:A:GLU:H  | 1:10:A:ILE:HG22 | 37       | 0.29          |
| (1,199)  | 1:90:A:GLU:H  | 1:10:A:ILE:HG23 | 37       | 0.29          |
| (1,176)  | 1:10:A:ILE:H  | 1:35:A:PHE:HD1  | 12       | 0.29          |
| (1,176)  | 1:10:A:ILE:H  | 1:35:A:PHE:HD2  | 12       | 0.29          |
| (1,176)  | 1:10:A:ILE:H  | 1:35:A:PHE:HD1  | 19       | 0.29          |
| (1,176)  | 1:10:A:ILE:H  | 1:35:A:PHE:HD2  | 19       | 0.29          |
| (1,176)  | 1:10:A:ILE:H  | 1:35:A:PHE:HD1  | 21       | 0.29          |
| (1,176)  | 1:10:A:ILE:H  | 1:35:A:PHE:HD2  | 21       | 0.29          |
| (1,149)  | 1:45:A:GLY:H  | 1:46:A:PRO:HD3  | 13       | 0.29          |
| (1,123)  | 1:55:A:TYR:H  | 1:54:A:LYS:H    | 6        | 0.29          |
| (1,123)  | 1:55:A:TYR:H  | 1:54:A:LYS:H    | 10       | 0.29          |
| (1,123)  | 1:55:A:TYR:H  | 1:54:A:LYS:H    | 11       | 0.29          |
| (1,123)  | 1:55:A:TYR:H  | 1:54:A:LYS:H    | 13       | 0.29          |
| (1,123)  | 1:55:A:TYR:H  | 1:54:A:LYS:H    | 15       | 0.29          |
| (1,123)  | 1:55:A:TYR:H  | 1:54:A:LYS:H    | 17       | 0.29          |
| (1,123)  | 1:55:A:TYR:H  | 1:54:A:LYS:H    | 20       | 0.29          |
| (1,123)  | 1:55:A:TYR:H  | 1:54:A:LYS:H    | 29       | 0.29          |
| (1,123)  | 1:55:A:TYR:H  | 1:54:A:LYS:H    | 33       | 0.29          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1   | 1        | 0.28          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2   | 1        | 0.28          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1   | 1        | 0.28          |
| (3,3176) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2   | 1        | 0.28          |
| (3,3176) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1   | 23       | 0.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,3176) | 1:5:A:PHE:HD1   | 1:5:A:PHE:HE2   | 23       | 0.28          |
| (3,3176) | 1:5:A:PHE:HD2   | 1:5:A:PHE:HE1   | 23       | 0.28          |
| (3,3176) | 1:5:A:PHE:HD2   | 1:5:A:PHE:HE2   | 23       | 0.28          |
| (3,3176) | 1:5:A:PHE:HD1   | 1:5:A:PHE:HE1   | 40       | 0.28          |
| (3,3176) | 1:5:A:PHE:HD1   | 1:5:A:PHE:HE2   | 40       | 0.28          |
| (3,3176) | 1:5:A:PHE:HD2   | 1:5:A:PHE:HE1   | 40       | 0.28          |
| (3,3176) | 1:5:A:PHE:HD2   | 1:5:A:PHE:HE2   | 40       | 0.28          |
| (3,3133) | 1:55:A:TYR:HD1  | 1:49:A:LEU:HB2  | 19       | 0.28          |
| (3,3133) | 1:55:A:TYR:HD2  | 1:49:A:LEU:HB2  | 19       | 0.28          |
| (3,2935) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 18       | 0.28          |
| (3,2925) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 18       | 0.28          |
| (3,2925) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 20       | 0.28          |
| (3,2925) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 35       | 0.28          |
| (3,2925) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 40       | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 1        | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 2        | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 3        | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 4        | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 5        | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 6        | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 7        | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 8        | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 9        | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 10       | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 11       | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 15       | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 16       | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 17       | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 18       | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 19       | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 20       | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 21       | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 23       | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 24       | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 25       | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 26       | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 27       | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 28       | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 29       | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 30       | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 31       | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 32       | 0.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 33       | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 34       | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 36       | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 37       | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 38       | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 39       | 0.28          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 40       | 0.28          |
| (3,2763) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 2        | 0.28          |
| (3,2763) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 11       | 0.28          |
| (3,2763) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 13       | 0.28          |
| (3,2763) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 14       | 0.28          |
| (3,2763) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 15       | 0.28          |
| (3,2763) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 17       | 0.28          |
| (3,2763) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 18       | 0.28          |
| (3,2763) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 21       | 0.28          |
| (3,2763) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 22       | 0.28          |
| (3,2763) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 23       | 0.28          |
| (3,2763) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 24       | 0.28          |
| (3,2763) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 25       | 0.28          |
| (3,2763) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 27       | 0.28          |
| (3,2763) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 28       | 0.28          |
| (3,2763) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 29       | 0.28          |
| (3,2763) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 30       | 0.28          |
| (3,2763) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 32       | 0.28          |
| (3,2763) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 34       | 0.28          |
| (3,2763) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 35       | 0.28          |
| (3,2763) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 39       | 0.28          |
| (3,2763) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 40       | 0.28          |
| (3,2656) | 1:17:A:GLN:HB3  | 1:17:A:GLN:HG2  | 8        | 0.28          |
| (3,2485) | 1:9:A:PRO:HD3   | 1:9:A:PRO:HB3   | 33       | 0.28          |
| (3,2440) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 2        | 0.28          |
| (3,2440) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 11       | 0.28          |
| (3,2440) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 13       | 0.28          |
| (3,2440) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 14       | 0.28          |
| (3,2440) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 15       | 0.28          |
| (3,2440) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 17       | 0.28          |
| (3,2440) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 18       | 0.28          |
| (3,2440) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 21       | 0.28          |
| (3,2440) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 22       | 0.28          |
| (3,2440) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 23       | 0.28          |
| (3,2440) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 24       | 0.28          |
| (3,2440) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 25       | 0.28          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2440) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3 | 27       | 0.28          |
| (3,2440) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3 | 28       | 0.28          |
| (3,2440) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3 | 29       | 0.28          |
| (3,2440) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3 | 30       | 0.28          |
| (3,2440) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3 | 32       | 0.28          |
| (3,2440) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3 | 34       | 0.28          |
| (3,2440) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3 | 35       | 0.28          |
| (3,2440) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3 | 39       | 0.28          |
| (3,2440) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3 | 40       | 0.28          |
| (3,2288) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H   | 6        | 0.28          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 1        | 0.28          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 1        | 0.28          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 1        | 0.28          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 2        | 0.28          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 2        | 0.28          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 2        | 0.28          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 4        | 0.28          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 4        | 0.28          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 4        | 0.28          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 5        | 0.28          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 5        | 0.28          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 5        | 0.28          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 9        | 0.28          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 9        | 0.28          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 9        | 0.28          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 17       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 17       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 17       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 18       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 18       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 18       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 19       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 19       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 19       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 21       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 21       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 21       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 23       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 23       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 23       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 24       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 24       | 0.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 24       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 25       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 25       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 25       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 28       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 28       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 28       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 30       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 30       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 30       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 31       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 31       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 31       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 33       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 33       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 33       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 36       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 36       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 36       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 38       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 38       | 0.28          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 38       | 0.28          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 3        | 0.28          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 3        | 0.28          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 3        | 0.28          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 6        | 0.28          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 6        | 0.28          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 6        | 0.28          |
| (3,1539) | 1:2:A:ILE:HD11  | 1:2:A:ILE:HA    | 13       | 0.28          |
| (3,1539) | 1:2:A:ILE:HD12  | 1:2:A:ILE:HA    | 13       | 0.28          |
| (3,1539) | 1:2:A:ILE:HD13  | 1:2:A:ILE:HA    | 13       | 0.28          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 28       | 0.28          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H    | 5        | 0.28          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H    | 5        | 0.28          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H    | 5        | 0.28          |
| (3,1188) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 28       | 0.28          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 1        | 0.28          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 1        | 0.28          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD23 | 1        | 0.28          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 2        | 0.28          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 2        | 0.28          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD23 | 2        | 0.28          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 4        | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 4        | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 4        | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 5        | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 5        | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 5        | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 9        | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 9        | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 9        | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 17       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 17       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 17       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 18       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 18       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 18       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 19       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 19       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 19       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 21       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 21       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 21       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 23       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 23       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 23       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 24       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 24       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 24       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 25       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 25       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 25       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 28       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 28       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 28       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 30       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 30       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 30       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 31       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 31       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 31       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 33       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 33       | 0.28          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 33       | 0.28          |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (3,935)  | 1:98:A:LYS:H  | 1:97:A:LEU:HD21 | 36       | 0.28          |
| (3,935)  | 1:98:A:LYS:H  | 1:97:A:LEU:HD22 | 36       | 0.28          |
| (3,935)  | 1:98:A:LYS:H  | 1:97:A:LEU:HD23 | 36       | 0.28          |
| (3,935)  | 1:98:A:LYS:H  | 1:97:A:LEU:HD21 | 38       | 0.28          |
| (3,935)  | 1:98:A:LYS:H  | 1:97:A:LEU:HD22 | 38       | 0.28          |
| (3,935)  | 1:98:A:LYS:H  | 1:97:A:LEU:HD23 | 38       | 0.28          |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 5        | 0.28          |
| (3,584)  | 1:93:A:SER:H  | 1:92:A:ARG:HB2  | 2        | 0.28          |
| (3,584)  | 1:93:A:SER:H  | 1:92:A:ARG:HB2  | 5        | 0.28          |
| (3,584)  | 1:93:A:SER:H  | 1:92:A:ARG:HB2  | 8        | 0.28          |
| (3,584)  | 1:93:A:SER:H  | 1:92:A:ARG:HB2  | 14       | 0.28          |
| (3,584)  | 1:93:A:SER:H  | 1:92:A:ARG:HB2  | 15       | 0.28          |
| (3,584)  | 1:93:A:SER:H  | 1:92:A:ARG:HB2  | 17       | 0.28          |
| (3,584)  | 1:93:A:SER:H  | 1:92:A:ARG:HB2  | 21       | 0.28          |
| (3,584)  | 1:93:A:SER:H  | 1:92:A:ARG:HB2  | 23       | 0.28          |
| (3,584)  | 1:93:A:SER:H  | 1:92:A:ARG:HB2  | 24       | 0.28          |
| (3,584)  | 1:93:A:SER:H  | 1:92:A:ARG:HB2  | 30       | 0.28          |
| (3,584)  | 1:93:A:SER:H  | 1:92:A:ARG:HB2  | 34       | 0.28          |
| (3,584)  | 1:93:A:SER:H  | 1:92:A:ARG:HB2  | 37       | 0.28          |
| (3,584)  | 1:93:A:SER:H  | 1:92:A:ARG:HB2  | 39       | 0.28          |
| (3,584)  | 1:93:A:SER:H  | 1:92:A:ARG:HB2  | 40       | 0.28          |
| (3,176)  | 1:10:A:ILE:H  | 1:35:A:PHE:HD1  | 28       | 0.28          |
| (3,176)  | 1:10:A:ILE:H  | 1:35:A:PHE:HD2  | 28       | 0.28          |
| (3,176)  | 1:10:A:ILE:H  | 1:35:A:PHE:HD1  | 29       | 0.28          |
| (3,176)  | 1:10:A:ILE:H  | 1:35:A:PHE:HD2  | 29       | 0.28          |
| (3,176)  | 1:10:A:ILE:H  | 1:35:A:PHE:HD1  | 34       | 0.28          |
| (3,176)  | 1:10:A:ILE:H  | 1:35:A:PHE:HD2  | 34       | 0.28          |
| (3,176)  | 1:10:A:ILE:H  | 1:35:A:PHE:HD1  | 37       | 0.28          |
| (3,176)  | 1:10:A:ILE:H  | 1:35:A:PHE:HD2  | 37       | 0.28          |
| (3,125)  | 1:55:A:TYR:H  | 1:54:A:LYS:H    | 24       | 0.28          |
| (3,125)  | 1:55:A:TYR:H  | 1:54:A:LYS:H    | 30       | 0.28          |
| (3,125)  | 1:55:A:TYR:H  | 1:54:A:LYS:H    | 40       | 0.28          |
| (3,22)   | 1:89:A:GLY:H  | 1:85:A:LEU:H    | 36       | 0.28          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1   | 1        | 0.28          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2   | 1        | 0.28          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1   | 1        | 0.28          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2   | 1        | 0.28          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1   | 23       | 0.28          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE2   | 23       | 0.28          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE1   | 23       | 0.28          |
| (1,3170) | 1:5:A:PHE:HD2 | 1:5:A:PHE:HE2   | 23       | 0.28          |
| (1,3170) | 1:5:A:PHE:HD1 | 1:5:A:PHE:HE1   | 40       | 0.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3170) | 1:5:A:PHE:HD1   | 1:5:A:PHE:HE2   | 40       | 0.28          |
| (1,3170) | 1:5:A:PHE:HD2   | 1:5:A:PHE:HE1   | 40       | 0.28          |
| (1,3170) | 1:5:A:PHE:HD2   | 1:5:A:PHE:HE2   | 40       | 0.28          |
| (1,3127) | 1:55:A:TYR:HD1  | 1:49:A:LEU:HB2  | 19       | 0.28          |
| (1,3127) | 1:55:A:TYR:HD2  | 1:49:A:LEU:HB2  | 19       | 0.28          |
| (1,2928) | 1:11:A:GLN:HG3  | 1:11:A:GLN:HB3  | 18       | 0.28          |
| (1,2918) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 18       | 0.28          |
| (1,2918) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 20       | 0.28          |
| (1,2918) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 35       | 0.28          |
| (1,2918) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 40       | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 1        | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 2        | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 3        | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 4        | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 5        | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 6        | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 7        | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 8        | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 9        | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 10       | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 11       | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 15       | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 16       | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 17       | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 18       | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 19       | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 20       | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 21       | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 23       | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 24       | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 25       | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 26       | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 27       | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 28       | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 29       | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 30       | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 31       | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 32       | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 33       | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 34       | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 36       | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 37       | 0.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 38       | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 39       | 0.28          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 40       | 0.28          |
| (1,2756) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 2        | 0.28          |
| (1,2756) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 11       | 0.28          |
| (1,2756) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 13       | 0.28          |
| (1,2756) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 14       | 0.28          |
| (1,2756) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 15       | 0.28          |
| (1,2756) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 17       | 0.28          |
| (1,2756) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 18       | 0.28          |
| (1,2756) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 21       | 0.28          |
| (1,2756) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 22       | 0.28          |
| (1,2756) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 23       | 0.28          |
| (1,2756) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 24       | 0.28          |
| (1,2756) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 25       | 0.28          |
| (1,2756) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 27       | 0.28          |
| (1,2756) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 28       | 0.28          |
| (1,2756) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 29       | 0.28          |
| (1,2756) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 30       | 0.28          |
| (1,2756) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 32       | 0.28          |
| (1,2756) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 34       | 0.28          |
| (1,2756) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 35       | 0.28          |
| (1,2756) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 39       | 0.28          |
| (1,2756) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 40       | 0.28          |
| (1,2652) | 1:17:A:GLN:HB3  | 1:17:A:GLN:HG2  | 8        | 0.28          |
| (1,2437) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 2        | 0.28          |
| (1,2437) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 11       | 0.28          |
| (1,2437) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 13       | 0.28          |
| (1,2437) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 14       | 0.28          |
| (1,2437) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 15       | 0.28          |
| (1,2437) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 17       | 0.28          |
| (1,2437) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 18       | 0.28          |
| (1,2437) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 21       | 0.28          |
| (1,2437) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 22       | 0.28          |
| (1,2437) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 23       | 0.28          |
| (1,2437) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 24       | 0.28          |
| (1,2437) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 25       | 0.28          |
| (1,2437) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 27       | 0.28          |
| (1,2437) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 28       | 0.28          |
| (1,2437) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 29       | 0.28          |
| (1,2437) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 30       | 0.28          |
| (1,2437) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 32       | 0.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2437) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 34       | 0.28          |
| (1,2437) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 35       | 0.28          |
| (1,2437) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 39       | 0.28          |
| (1,2437) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 40       | 0.28          |
| (1,2285) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H    | 6        | 0.28          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 11       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 11       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 11       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 11       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 11       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 11       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 11       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 11       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 11       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 22       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 22       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 22       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 22       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 22       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 22       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 22       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 22       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 22       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 25       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 25       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 25       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 25       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 25       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 25       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 25       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 25       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 25       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 34       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 34       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 34       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 34       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 34       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 34       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 34       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 34       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 34       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 39       | 0.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 39       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 39       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 39       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 39       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 39       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 39       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 39       | 0.28          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 39       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 1        | 0.28          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 1        | 0.28          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 1        | 0.28          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 2        | 0.28          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 2        | 0.28          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 2        | 0.28          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 4        | 0.28          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 4        | 0.28          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 4        | 0.28          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 5        | 0.28          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 5        | 0.28          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 5        | 0.28          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 9        | 0.28          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 9        | 0.28          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 9        | 0.28          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 17       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 17       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 17       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 18       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 18       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 18       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 19       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 19       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 19       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 21       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 21       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 21       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 23       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 23       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 23       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 24       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 24       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 24       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 25       | 0.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 25       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 25       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 28       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 28       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 28       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 30       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 30       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 30       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 31       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 31       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 31       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 33       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 33       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 33       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 36       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 36       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 36       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 38       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 38       | 0.28          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 38       | 0.28          |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 3        | 0.28          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 3        | 0.28          |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 3        | 0.28          |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 6        | 0.28          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 6        | 0.28          |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 6        | 0.28          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3  | 38       | 0.28          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3  | 38       | 0.28          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3  | 38       | 0.28          |
| (1,1535) | 1:2:A:ILE:HD11  | 1:2:A:ILE:HA    | 13       | 0.28          |
| (1,1535) | 1:2:A:ILE:HD12  | 1:2:A:ILE:HA    | 13       | 0.28          |
| (1,1535) | 1:2:A:ILE:HD13  | 1:2:A:ILE:HA    | 13       | 0.28          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 28       | 0.28          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H    | 5        | 0.28          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H    | 5        | 0.28          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H    | 5        | 0.28          |
| (1,1184) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 28       | 0.28          |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 1        | 0.28          |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 1        | 0.28          |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD23 | 1        | 0.28          |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 2        | 0.28          |
| (1,934)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 2        | 0.28          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 2        | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 4        | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 4        | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 4        | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 5        | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 5        | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 5        | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 9        | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 9        | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 9        | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 17       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 17       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 17       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 18       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 18       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 18       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 19       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 19       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 19       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 21       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 21       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 21       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 23       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 23       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 23       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 24       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 24       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 24       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 25       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 25       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 25       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 28       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 28       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 28       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 30       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 30       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 30       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 31       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 31       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 31       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 33       | 0.28          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 33       | 0.28          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,934)  | 1:98:A:LYS:H   | 1:97:A:LEU:HD23 | 33       | 0.28          |
| (1,934)  | 1:98:A:LYS:H   | 1:97:A:LEU:HD21 | 36       | 0.28          |
| (1,934)  | 1:98:A:LYS:H   | 1:97:A:LEU:HD22 | 36       | 0.28          |
| (1,934)  | 1:98:A:LYS:H   | 1:97:A:LEU:HD23 | 36       | 0.28          |
| (1,934)  | 1:98:A:LYS:H   | 1:97:A:LEU:HD21 | 38       | 0.28          |
| (1,934)  | 1:98:A:LYS:H   | 1:97:A:LEU:HD22 | 38       | 0.28          |
| (1,934)  | 1:98:A:LYS:H   | 1:97:A:LEU:HD23 | 38       | 0.28          |
| (1,932)  | 1:98:A:LYS:H   | 1:19:A:ILE:HB   | 5        | 0.28          |
| (1,584)  | 1:93:A:SER:H   | 1:92:A:ARG:HB2  | 2        | 0.28          |
| (1,584)  | 1:93:A:SER:H   | 1:92:A:ARG:HB2  | 5        | 0.28          |
| (1,584)  | 1:93:A:SER:H   | 1:92:A:ARG:HB2  | 8        | 0.28          |
| (1,584)  | 1:93:A:SER:H   | 1:92:A:ARG:HB2  | 14       | 0.28          |
| (1,584)  | 1:93:A:SER:H   | 1:92:A:ARG:HB2  | 15       | 0.28          |
| (1,584)  | 1:93:A:SER:H   | 1:92:A:ARG:HB2  | 17       | 0.28          |
| (1,584)  | 1:93:A:SER:H   | 1:92:A:ARG:HB2  | 21       | 0.28          |
| (1,584)  | 1:93:A:SER:H   | 1:92:A:ARG:HB2  | 23       | 0.28          |
| (1,584)  | 1:93:A:SER:H   | 1:92:A:ARG:HB2  | 24       | 0.28          |
| (1,584)  | 1:93:A:SER:H   | 1:92:A:ARG:HB2  | 30       | 0.28          |
| (1,584)  | 1:93:A:SER:H   | 1:92:A:ARG:HB2  | 34       | 0.28          |
| (1,584)  | 1:93:A:SER:H   | 1:92:A:ARG:HB2  | 37       | 0.28          |
| (1,584)  | 1:93:A:SER:H   | 1:92:A:ARG:HB2  | 39       | 0.28          |
| (1,584)  | 1:93:A:SER:H   | 1:92:A:ARG:HB2  | 40       | 0.28          |
| (1,199)  | 1:90:A:GLU:H   | 1:10:A:ILE:HG21 | 36       | 0.28          |
| (1,199)  | 1:90:A:GLU:H   | 1:10:A:ILE:HG22 | 36       | 0.28          |
| (1,199)  | 1:90:A:GLU:H   | 1:10:A:ILE:HG23 | 36       | 0.28          |
| (1,176)  | 1:10:A:ILE:H   | 1:35:A:PHE:HD1  | 28       | 0.28          |
| (1,176)  | 1:10:A:ILE:H   | 1:35:A:PHE:HD2  | 28       | 0.28          |
| (1,176)  | 1:10:A:ILE:H   | 1:35:A:PHE:HD1  | 29       | 0.28          |
| (1,176)  | 1:10:A:ILE:H   | 1:35:A:PHE:HD2  | 29       | 0.28          |
| (1,176)  | 1:10:A:ILE:H   | 1:35:A:PHE:HD1  | 34       | 0.28          |
| (1,176)  | 1:10:A:ILE:H   | 1:35:A:PHE:HD2  | 34       | 0.28          |
| (1,176)  | 1:10:A:ILE:H   | 1:35:A:PHE:HD1  | 37       | 0.28          |
| (1,176)  | 1:10:A:ILE:H   | 1:35:A:PHE:HD2  | 37       | 0.28          |
| (1,149)  | 1:45:A:GLY:H   | 1:46:A:PRO:HD3  | 6        | 0.28          |
| (1,149)  | 1:45:A:GLY:H   | 1:46:A:PRO:HD3  | 15       | 0.28          |
| (1,149)  | 1:45:A:GLY:H   | 1:46:A:PRO:HD3  | 17       | 0.28          |
| (1,123)  | 1:55:A:TYR:H   | 1:54:A:LYS:H    | 24       | 0.28          |
| (1,123)  | 1:55:A:TYR:H   | 1:54:A:LYS:H    | 30       | 0.28          |
| (1,123)  | 1:55:A:TYR:H   | 1:54:A:LYS:H    | 40       | 0.28          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 21       | 0.27          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 21       | 0.27          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 27       | 0.27          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,3218) | 1:65:A:TYR:HE2  | 1:58:A:ARG:HB3  | 27       | 0.27          |
| (3,3205) | 1:43:A:TYR:HD1  | 1:80:A:SER:HB2  | 28       | 0.27          |
| (3,3205) | 1:43:A:TYR:HD2  | 1:80:A:SER:HB2  | 28       | 0.27          |
| (3,3165) | 1:42:A:TRP:HD1  | 1:42:A:TRP:HB3  | 13       | 0.27          |
| (3,3165) | 1:42:A:TRP:HD1  | 1:42:A:TRP:HB3  | 38       | 0.27          |
| (3,3133) | 1:55:A:TYR:HD1  | 1:49:A:LEU:HB2  | 29       | 0.27          |
| (3,3133) | 1:55:A:TYR:HD2  | 1:49:A:LEU:HB2  | 29       | 0.27          |
| (3,3056) | 1:60:A:ASP:HB2  | 1:63:A:CYS:HB2  | 29       | 0.27          |
| (3,3055) | 1:57:A:PHE:HB3  | 1:42:A:TRP:HE1  | 12       | 0.27          |
| (3,3055) | 1:57:A:PHE:HB3  | 1:42:A:TRP:HE1  | 16       | 0.27          |
| (3,2925) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 1        | 0.27          |
| (3,2925) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 4        | 0.27          |
| (3,2925) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 11       | 0.27          |
| (3,2925) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 14       | 0.27          |
| (3,2925) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 32       | 0.27          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 12       | 0.27          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 14       | 0.27          |
| (3,2788) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 22       | 0.27          |
| (3,2763) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 19       | 0.27          |
| (3,2763) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 31       | 0.27          |
| (3,2653) | 1:17:A:GLN:HB2  | 1:18:A:ASN:H    | 37       | 0.27          |
| (3,2470) | 1:4:A:PRO:HB2   | 1:4:A:PRO:HD2   | 1        | 0.27          |
| (3,2470) | 1:4:A:PRO:HB2   | 1:4:A:PRO:HD2   | 10       | 0.27          |
| (3,2440) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 19       | 0.27          |
| (3,2440) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 31       | 0.27          |
| (3,2288) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H    | 1        | 0.27          |
| (3,2288) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H    | 8        | 0.27          |
| (3,2288) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H    | 9        | 0.27          |
| (3,2288) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H    | 13       | 0.27          |
| (3,2288) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H    | 15       | 0.27          |
| (3,2288) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H    | 23       | 0.27          |
| (3,2288) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H    | 29       | 0.27          |
| (3,2288) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H    | 33       | 0.27          |
| (3,2288) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H    | 37       | 0.27          |
| (3,2288) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H    | 40       | 0.27          |
| (3,2216) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1  | 13       | 0.27          |
| (3,2216) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1  | 38       | 0.27          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA   | 5        | 0.27          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA   | 5        | 0.27          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA   | 5        | 0.27          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA   | 15       | 0.27          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA   | 15       | 0.27          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 15       | 0.27          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 35       | 0.27          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 35       | 0.27          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 35       | 0.27          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 30       | 0.27          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 30       | 0.27          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 30       | 0.27          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 30       | 0.27          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 30       | 0.27          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 30       | 0.27          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 16       | 0.27          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 16       | 0.27          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 16       | 0.27          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 1        | 0.27          |
| (3,1781) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H   | 6        | 0.27          |
| (3,1781) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H   | 7        | 0.27          |
| (3,1781) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H   | 12       | 0.27          |
| (3,1781) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H   | 13       | 0.27          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 10       | 0.27          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 10       | 0.27          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 10       | 0.27          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 13       | 0.27          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 13       | 0.27          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 13       | 0.27          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 16       | 0.27          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 16       | 0.27          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 16       | 0.27          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 20       | 0.27          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 20       | 0.27          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 20       | 0.27          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 22       | 0.27          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 22       | 0.27          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 22       | 0.27          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 27       | 0.27          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 27       | 0.27          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 27       | 0.27          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 35       | 0.27          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 35       | 0.27          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 35       | 0.27          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 39       | 0.27          |
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H   | 39       | 0.27          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H   | 39       | 0.27          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 9        | 0.27          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 9        | 0.27          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 9        | 0.27          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 12       | 0.27          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 12       | 0.27          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 12       | 0.27          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 16       | 0.27          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 16       | 0.27          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 16       | 0.27          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 19       | 0.27          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 19       | 0.27          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 19       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 3        | 0.27          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 3        | 0.27          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 3        | 0.27          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 4        | 0.27          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 4        | 0.27          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 4        | 0.27          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 5        | 0.27          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 5        | 0.27          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 5        | 0.27          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 6        | 0.27          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 6        | 0.27          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 6        | 0.27          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 7        | 0.27          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 7        | 0.27          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 7        | 0.27          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 8        | 0.27          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 8        | 0.27          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 8        | 0.27          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 9        | 0.27          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 9        | 0.27          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 9        | 0.27          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 10       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 10       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 10       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 12       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 12       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 12       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 13       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 13       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 13       | 0.27          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 16       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 16       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 16       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 18       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 18       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 18       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 20       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 20       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 20       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 24       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 24       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 24       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 26       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 26       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 26       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 29       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 29       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 29       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 32       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 32       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 32       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 33       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 33       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 33       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 35       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 35       | 0.27          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 35       | 0.27          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H    | 34       | 0.27          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H    | 34       | 0.27          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H    | 34       | 0.27          |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H    | 28       | 0.27          |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H    | 28       | 0.27          |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H    | 28       | 0.27          |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 8        | 0.27          |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 20       | 0.27          |
| (3,1188) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 1        | 0.27          |
| (3,1188) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 8        | 0.27          |
| (3,1188) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 36       | 0.27          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 10       | 0.27          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD22 | 10       | 0.27          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD23 | 10       | 0.27          |
| (3,935)  | 1:98:A:LYS:H    | 1:97:A:LEU:HD21 | 13       | 0.27          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 13       | 0.27          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 13       | 0.27          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 16       | 0.27          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 16       | 0.27          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 16       | 0.27          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 20       | 0.27          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 20       | 0.27          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 20       | 0.27          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 22       | 0.27          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 22       | 0.27          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 22       | 0.27          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 27       | 0.27          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 27       | 0.27          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 27       | 0.27          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 35       | 0.27          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 35       | 0.27          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 35       | 0.27          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 39       | 0.27          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 39       | 0.27          |
| (3,935) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 39       | 0.27          |
| (3,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 37       | 0.27          |
| (3,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 9        | 0.27          |
| (3,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 34       | 0.27          |
| (3,584) | 1:93:A:SER:H | 1:92:A:ARG:HB2  | 3        | 0.27          |
| (3,584) | 1:93:A:SER:H | 1:92:A:ARG:HB2  | 4        | 0.27          |
| (3,584) | 1:93:A:SER:H | 1:92:A:ARG:HB2  | 7        | 0.27          |
| (3,584) | 1:93:A:SER:H | 1:92:A:ARG:HB2  | 10       | 0.27          |
| (3,584) | 1:93:A:SER:H | 1:92:A:ARG:HB2  | 13       | 0.27          |
| (3,584) | 1:93:A:SER:H | 1:92:A:ARG:HB2  | 20       | 0.27          |
| (3,584) | 1:93:A:SER:H | 1:92:A:ARG:HB2  | 35       | 0.27          |
| (3,584) | 1:93:A:SER:H | 1:92:A:ARG:HB2  | 36       | 0.27          |
| (3,584) | 1:93:A:SER:H | 1:92:A:ARG:HB2  | 38       | 0.27          |
| (3,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 20       | 0.27          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 22       | 0.27          |
| (3,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 37       | 0.27          |
| (3,365) | 1:18:A:ASN:H | 1:18:A:ASN:HB2  | 37       | 0.27          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 14       | 0.27          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 14       | 0.27          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 25       | 0.27          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 25       | 0.27          |
| (3,125) | 1:55:A:TYR:H | 1:54:A:LYS:H    | 4        | 0.27          |
| (3,125) | 1:55:A:TYR:H | 1:54:A:LYS:H    | 27       | 0.27          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,125)  | 1:55:A:TYR:H    | 1:54:A:LYS:H    | 39       | 0.27          |
| (1,3212) | 1:65:A:TYR:HE1  | 1:58:A:ARG:HB3  | 21       | 0.27          |
| (1,3212) | 1:65:A:TYR:HE2  | 1:58:A:ARG:HB3  | 21       | 0.27          |
| (1,3212) | 1:65:A:TYR:HE1  | 1:58:A:ARG:HB3  | 27       | 0.27          |
| (1,3212) | 1:65:A:TYR:HE2  | 1:58:A:ARG:HB3  | 27       | 0.27          |
| (1,3199) | 1:43:A:TYR:HD1  | 1:80:A:SER:HB2  | 28       | 0.27          |
| (1,3199) | 1:43:A:TYR:HD2  | 1:80:A:SER:HB2  | 28       | 0.27          |
| (1,3159) | 1:42:A:TRP:HD1  | 1:42:A:TRP:HB3  | 13       | 0.27          |
| (1,3159) | 1:42:A:TRP:HD1  | 1:42:A:TRP:HB3  | 38       | 0.27          |
| (1,3127) | 1:55:A:TYR:HD1  | 1:49:A:LEU:HB2  | 29       | 0.27          |
| (1,3127) | 1:55:A:TYR:HD2  | 1:49:A:LEU:HB2  | 29       | 0.27          |
| (1,3048) | 1:60:A:ASP:HB2  | 1:63:A:CYS:HB2  | 29       | 0.27          |
| (1,3047) | 1:57:A:PHE:HB3  | 1:42:A:TRP:HE1  | 12       | 0.27          |
| (1,3047) | 1:57:A:PHE:HB3  | 1:42:A:TRP:HE1  | 16       | 0.27          |
| (1,2918) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 1        | 0.27          |
| (1,2918) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 4        | 0.27          |
| (1,2918) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 11       | 0.27          |
| (1,2918) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 14       | 0.27          |
| (1,2918) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 32       | 0.27          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 12       | 0.27          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 14       | 0.27          |
| (1,2781) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HB3 | 22       | 0.27          |
| (1,2756) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 19       | 0.27          |
| (1,2756) | 1:90:A:GLU:HG3  | 1:90:A:GLU:HA   | 31       | 0.27          |
| (1,2649) | 1:17:A:GLN:HB2  | 1:18:A:ASN:H    | 37       | 0.27          |
| (1,2467) | 1:4:A:PRO:HB2   | 1:4:A:PRO:HD2   | 1        | 0.27          |
| (1,2467) | 1:4:A:PRO:HB2   | 1:4:A:PRO:HD2   | 10       | 0.27          |
| (1,2437) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 19       | 0.27          |
| (1,2437) | 1:90:A:GLU:HA   | 1:90:A:GLU:HG3  | 31       | 0.27          |
| (1,2285) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H    | 1        | 0.27          |
| (1,2285) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H    | 8        | 0.27          |
| (1,2285) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H    | 9        | 0.27          |
| (1,2285) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H    | 13       | 0.27          |
| (1,2285) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H    | 15       | 0.27          |
| (1,2285) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H    | 23       | 0.27          |
| (1,2285) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H    | 29       | 0.27          |
| (1,2285) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H    | 33       | 0.27          |
| (1,2285) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H    | 37       | 0.27          |
| (1,2285) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H    | 40       | 0.27          |
| (1,2213) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1  | 13       | 0.27          |
| (1,2213) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1  | 38       | 0.27          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA   | 5        | 0.27          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA   | 5        | 0.27          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA   | 5        | 0.27          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA   | 15       | 0.27          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA   | 15       | 0.27          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA   | 15       | 0.27          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA   | 35       | 0.27          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA   | 35       | 0.27          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA   | 35       | 0.27          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1  | 30       | 0.27          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2  | 30       | 0.27          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1  | 30       | 0.27          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2  | 30       | 0.27          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1  | 30       | 0.27          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2  | 30       | 0.27          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 16       | 0.27          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 16       | 0.27          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 16       | 0.27          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 1        | 0.27          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 1        | 0.27          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 1        | 0.27          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 1        | 0.27          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 1        | 0.27          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 1        | 0.27          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 1        | 0.27          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 1        | 0.27          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 1        | 0.27          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 1        | 0.27          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 19       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 19       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 19       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 19       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 19       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 19       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 19       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 19       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 19       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 20       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 20       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 20       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 20       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 20       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 20       | 0.27          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 20       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 20       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 20       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 21       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 21       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 21       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 21       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 21       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 21       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 21       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 21       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 21       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 27       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 27       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 27       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 27       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 27       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 27       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 27       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 27       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 27       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 33       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 33       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 33       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 33       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 33       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 33       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 33       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 33       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 33       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 36       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 36       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 36       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 36       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 36       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 36       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 36       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 36       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 36       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 38       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 38       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 38       | 0.27          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 38       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 38       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 38       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 38       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 38       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 38       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 40       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 40       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 40       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 40       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 40       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 40       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 40       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 40       | 0.27          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 40       | 0.27          |
| (1,1778) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H    | 6        | 0.27          |
| (1,1778) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H    | 7        | 0.27          |
| (1,1778) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H    | 12       | 0.27          |
| (1,1778) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H    | 13       | 0.27          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 10       | 0.27          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 10       | 0.27          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 10       | 0.27          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 13       | 0.27          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 13       | 0.27          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 13       | 0.27          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 16       | 0.27          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 16       | 0.27          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 16       | 0.27          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 20       | 0.27          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 20       | 0.27          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 20       | 0.27          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 22       | 0.27          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 22       | 0.27          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 22       | 0.27          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 27       | 0.27          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 27       | 0.27          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 27       | 0.27          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 35       | 0.27          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 35       | 0.27          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 35       | 0.27          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 39       | 0.27          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 39       | 0.27          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 39       | 0.27          |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 9        | 0.27          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 9        | 0.27          |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 9        | 0.27          |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 12       | 0.27          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 12       | 0.27          |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 12       | 0.27          |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 16       | 0.27          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 16       | 0.27          |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 16       | 0.27          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3  | 32       | 0.27          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3  | 32       | 0.27          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3  | 32       | 0.27          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 19       | 0.27          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 19       | 0.27          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 19       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 3        | 0.27          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 3        | 0.27          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 3        | 0.27          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 4        | 0.27          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 4        | 0.27          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 4        | 0.27          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 5        | 0.27          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 5        | 0.27          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 5        | 0.27          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 6        | 0.27          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 6        | 0.27          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 6        | 0.27          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 7        | 0.27          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 7        | 0.27          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 7        | 0.27          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 8        | 0.27          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 8        | 0.27          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 8        | 0.27          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 9        | 0.27          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 9        | 0.27          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 9        | 0.27          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 10       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 10       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 10       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 12       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 12       | 0.27          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 12       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 13       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 13       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 13       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 16       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 16       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 16       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 18       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 18       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 18       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 20       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 20       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 20       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 24       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 24       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 24       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 26       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 26       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 26       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 29       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 29       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 29       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 32       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 32       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 32       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 33       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 33       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 33       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 35       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 35       | 0.27          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 35       | 0.27          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H    | 34       | 0.27          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H    | 34       | 0.27          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H    | 34       | 0.27          |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H    | 28       | 0.27          |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H    | 28       | 0.27          |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H    | 28       | 0.27          |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 8        | 0.27          |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 20       | 0.27          |
| (1,1184) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 1        | 0.27          |
| (1,1184) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 8        | 0.27          |
| (1,1184) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 36       | 0.27          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 10       | 0.27          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 10       | 0.27          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 10       | 0.27          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 13       | 0.27          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 13       | 0.27          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 13       | 0.27          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 16       | 0.27          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 16       | 0.27          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 16       | 0.27          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 20       | 0.27          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 20       | 0.27          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 20       | 0.27          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 22       | 0.27          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 22       | 0.27          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 22       | 0.27          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 27       | 0.27          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 27       | 0.27          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 27       | 0.27          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 35       | 0.27          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 35       | 0.27          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 35       | 0.27          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 39       | 0.27          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 39       | 0.27          |
| (1,934) | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 39       | 0.27          |
| (1,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 37       | 0.27          |
| (1,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 9        | 0.27          |
| (1,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 34       | 0.27          |
| (1,584) | 1:93:A:SER:H | 1:92:A:ARG:HB2  | 3        | 0.27          |
| (1,584) | 1:93:A:SER:H | 1:92:A:ARG:HB2  | 4        | 0.27          |
| (1,584) | 1:93:A:SER:H | 1:92:A:ARG:HB2  | 7        | 0.27          |
| (1,584) | 1:93:A:SER:H | 1:92:A:ARG:HB2  | 10       | 0.27          |
| (1,584) | 1:93:A:SER:H | 1:92:A:ARG:HB2  | 13       | 0.27          |
| (1,584) | 1:93:A:SER:H | 1:92:A:ARG:HB2  | 20       | 0.27          |
| (1,584) | 1:93:A:SER:H | 1:92:A:ARG:HB2  | 35       | 0.27          |
| (1,584) | 1:93:A:SER:H | 1:92:A:ARG:HB2  | 36       | 0.27          |
| (1,584) | 1:93:A:SER:H | 1:92:A:ARG:HB2  | 38       | 0.27          |
| (1,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 20       | 0.27          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 22       | 0.27          |
| (1,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 37       | 0.27          |
| (1,365) | 1:18:A:ASN:H | 1:18:A:ASN:HB2  | 37       | 0.27          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 14       | 0.27          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 14       | 0.27          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,176)  | 1:10:A:ILE:H   | 1:35:A:PHE:HD1 | 25       | 0.27          |
| (1,176)  | 1:10:A:ILE:H   | 1:35:A:PHE:HD2 | 25       | 0.27          |
| (1,149)  | 1:45:A:GLY:H   | 1:46:A:PRO:HD3 | 3        | 0.27          |
| (1,149)  | 1:45:A:GLY:H   | 1:46:A:PRO:HD3 | 20       | 0.27          |
| (1,123)  | 1:55:A:TYR:H   | 1:54:A:LYS:H   | 4        | 0.27          |
| (1,123)  | 1:55:A:TYR:H   | 1:54:A:LYS:H   | 27       | 0.27          |
| (1,123)  | 1:55:A:TYR:H   | 1:54:A:LYS:H   | 39       | 0.27          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3 | 23       | 0.26          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3 | 23       | 0.26          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3 | 24       | 0.26          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3 | 24       | 0.26          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3 | 33       | 0.26          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3 | 33       | 0.26          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3 | 38       | 0.26          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3 | 38       | 0.26          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3 | 39       | 0.26          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3 | 39       | 0.26          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 1        | 0.26          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 3        | 0.26          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 5        | 0.26          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 14       | 0.26          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 15       | 0.26          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 17       | 0.26          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 23       | 0.26          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 26       | 0.26          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 27       | 0.26          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 34       | 0.26          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 37       | 0.26          |
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2 | 7        | 0.26          |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2 | 7        | 0.26          |
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2 | 16       | 0.26          |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2 | 16       | 0.26          |
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2 | 39       | 0.26          |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2 | 39       | 0.26          |
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2 | 40       | 0.26          |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2 | 40       | 0.26          |
| (3,3056) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2 | 14       | 0.26          |
| (3,3056) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2 | 17       | 0.26          |
| (3,3056) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2 | 28       | 0.26          |
| (3,3056) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2 | 32       | 0.26          |
| (3,3056) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2 | 35       | 0.26          |
| (3,3056) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2 | 40       | 0.26          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1 | 15       | 0.26          |
| (3,2925) | 1:22:A:SER:HB2 | 1:25:A:GLN:H   | 2        | 0.26          |
| (3,2925) | 1:22:A:SER:HB2 | 1:25:A:GLN:H   | 12       | 0.26          |
| (3,2925) | 1:22:A:SER:HB2 | 1:25:A:GLN:H   | 19       | 0.26          |
| (3,2925) | 1:22:A:SER:HB2 | 1:25:A:GLN:H   | 21       | 0.26          |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 33       | 0.26          |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 35       | 0.26          |
| (3,2470) | 1:4:A:PRO:HB2  | 1:4:A:PRO:HD2  | 5        | 0.26          |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 17       | 0.26          |
| (3,2288) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 7        | 0.26          |
| (3,2288) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 10       | 0.26          |
| (3,2288) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 11       | 0.26          |
| (3,2288) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 12       | 0.26          |
| (3,2288) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 14       | 0.26          |
| (3,2288) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 16       | 0.26          |
| (3,2288) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 17       | 0.26          |
| (3,2288) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 20       | 0.26          |
| (3,2288) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 21       | 0.26          |
| (3,2288) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 22       | 0.26          |
| (3,2288) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 24       | 0.26          |
| (3,2288) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 25       | 0.26          |
| (3,2288) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 26       | 0.26          |
| (3,2288) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 27       | 0.26          |
| (3,2288) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 30       | 0.26          |
| (3,2288) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 31       | 0.26          |
| (3,2288) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 32       | 0.26          |
| (3,2288) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 34       | 0.26          |
| (3,2288) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 35       | 0.26          |
| (3,2288) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 36       | 0.26          |
| (3,2288) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 38       | 0.26          |
| (3,2288) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 39       | 0.26          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1 | 2        | 0.26          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2 | 2        | 0.26          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1 | 3        | 0.26          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2 | 3        | 0.26          |
| (3,2216) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 1        | 0.26          |
| (3,2216) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 3        | 0.26          |
| (3,2216) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 5        | 0.26          |
| (3,2216) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 14       | 0.26          |
| (3,2216) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 15       | 0.26          |
| (3,2216) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 17       | 0.26          |
| (3,2216) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 23       | 0.26          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2216) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 26       | 0.26          |
| (3,2216) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 27       | 0.26          |
| (3,2216) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 34       | 0.26          |
| (3,2216) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 37       | 0.26          |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H   | 27       | 0.26          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 2        | 0.26          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 2        | 0.26          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 2        | 0.26          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 8        | 0.26          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 8        | 0.26          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 8        | 0.26          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 13       | 0.26          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 13       | 0.26          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 13       | 0.26          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 17       | 0.26          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 17       | 0.26          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 17       | 0.26          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 20       | 0.26          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 20       | 0.26          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 20       | 0.26          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 21       | 0.26          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 21       | 0.26          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 21       | 0.26          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 11       | 0.26          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 11       | 0.26          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 11       | 0.26          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 11       | 0.26          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 11       | 0.26          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 11       | 0.26          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 14       | 0.26          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 14       | 0.26          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 14       | 0.26          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 14       | 0.26          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 14       | 0.26          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 14       | 0.26          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 38       | 0.26          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 38       | 0.26          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 38       | 0.26          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 38       | 0.26          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 38       | 0.26          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 38       | 0.26          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 1        | 0.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3  | 1        | 0.26          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3  | 1        | 0.26          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 4        | 0.26          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 5        | 0.26          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 6        | 0.26          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 7        | 0.26          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 8        | 0.26          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 9        | 0.26          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 10       | 0.26          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 13       | 0.26          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 19       | 0.26          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 21       | 0.26          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 22       | 0.26          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 23       | 0.26          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 25       | 0.26          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 29       | 0.26          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 30       | 0.26          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 31       | 0.26          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 32       | 0.26          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 36       | 0.26          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 38       | 0.26          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 39       | 0.26          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 40       | 0.26          |
| (3,1781) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H    | 9        | 0.26          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 7        | 0.26          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 7        | 0.26          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 7        | 0.26          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 20       | 0.26          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 20       | 0.26          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 20       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 1        | 0.26          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 1        | 0.26          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 1        | 0.26          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 2        | 0.26          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 2        | 0.26          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 2        | 0.26          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 11       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 11       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 11       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 14       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 14       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 14       | 0.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 15       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 15       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 15       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 17       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 17       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 17       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 19       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 19       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 19       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 21       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 21       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 21       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 22       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 22       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 22       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 23       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 23       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 23       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 25       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 25       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 25       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 27       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 27       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 27       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 28       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 28       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 28       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 30       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 30       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 30       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 31       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 31       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 31       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 34       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 34       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 34       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 36       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 36       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 36       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 37       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 37       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 37       | 0.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 38       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 38       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 38       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 39       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 39       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 39       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 40       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 40       | 0.26          |
| (3,1551) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 40       | 0.26          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 8        | 0.26          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 13       | 0.26          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 29       | 0.26          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 31       | 0.26          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 33       | 0.26          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 35       | 0.26          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H    | 26       | 0.26          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H    | 26       | 0.26          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H    | 26       | 0.26          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H    | 29       | 0.26          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H    | 29       | 0.26          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H    | 29       | 0.26          |
| (3,1188) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 2        | 0.26          |
| (3,1188) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 5        | 0.26          |
| (3,1188) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 9        | 0.26          |
| (3,1188) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 19       | 0.26          |
| (3,1188) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 23       | 0.26          |
| (3,1188) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 25       | 0.26          |
| (3,1188) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 29       | 0.26          |
| (3,1188) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 32       | 0.26          |
| (3,1188) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 40       | 0.26          |
| (3,1167) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 18       | 0.26          |
| (3,919)  | 1:37:A:ASP:H    | 1:36:A:ASP:HB3  | 33       | 0.26          |
| (3,919)  | 1:37:A:ASP:H    | 1:36:A:ASP:HB3  | 35       | 0.26          |
| (3,870)  | 1:8:A:GLU:H     | 1:9:A:PRO:HD2   | 10       | 0.26          |
| (3,849)  | 1:83:A:ALA:H    | 1:91:A:ALA:HB1  | 3        | 0.26          |
| (3,849)  | 1:83:A:ALA:H    | 1:91:A:ALA:HB2  | 3        | 0.26          |
| (3,849)  | 1:83:A:ALA:H    | 1:91:A:ALA:HB3  | 3        | 0.26          |
| (3,685)  | 1:23:A:GLU:H    | 1:23:A:GLU:HG3  | 6        | 0.26          |
| (3,685)  | 1:23:A:GLU:H    | 1:23:A:GLU:HG3  | 7        | 0.26          |
| (3,685)  | 1:23:A:GLU:H    | 1:23:A:GLU:HG3  | 13       | 0.26          |
| (3,685)  | 1:23:A:GLU:H    | 1:23:A:GLU:HG3  | 15       | 0.26          |
| (3,685)  | 1:23:A:GLU:H    | 1:23:A:GLU:HG3  | 19       | 0.26          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,685)  | 1:23:A:GLU:H   | 1:23:A:GLU:HG3  | 31       | 0.26          |
| (3,685)  | 1:23:A:GLU:H   | 1:23:A:GLU:HG3  | 40       | 0.26          |
| (3,584)  | 1:93:A:SER:H   | 1:92:A:ARG:HB2  | 9        | 0.26          |
| (3,584)  | 1:93:A:SER:H   | 1:92:A:ARG:HB2  | 12       | 0.26          |
| (3,584)  | 1:93:A:SER:H   | 1:92:A:ARG:HB2  | 19       | 0.26          |
| (3,584)  | 1:93:A:SER:H   | 1:92:A:ARG:HB2  | 26       | 0.26          |
| (3,546)  | 1:71:A:VAL:H   | 1:24:A:HIS:HA   | 5        | 0.26          |
| (3,546)  | 1:71:A:VAL:H   | 1:24:A:HIS:HA   | 10       | 0.26          |
| (3,525)  | 1:99:A:GLY:H   | 1:100:A:GLU:H   | 14       | 0.26          |
| (3,513)  | 1:67:A:THR:H   | 1:66:A:MET:HG3  | 10       | 0.26          |
| (3,513)  | 1:67:A:THR:H   | 1:66:A:MET:HG3  | 19       | 0.26          |
| (3,423)  | 1:69:A:HIS:H   | 1:69:A:HIS:HD2  | 6        | 0.26          |
| (3,423)  | 1:69:A:HIS:H   | 1:69:A:HIS:HD2  | 16       | 0.26          |
| (3,423)  | 1:69:A:HIS:H   | 1:69:A:HIS:HD2  | 18       | 0.26          |
| (3,343)  | 1:14:A:LYS:H   | 1:33:A:VAL:HA   | 3        | 0.26          |
| (3,343)  | 1:14:A:LYS:H   | 1:33:A:VAL:HA   | 17       | 0.26          |
| (3,343)  | 1:14:A:LYS:H   | 1:33:A:VAL:HA   | 27       | 0.26          |
| (3,176)  | 1:10:A:ILE:H   | 1:35:A:PHE:HD1  | 26       | 0.26          |
| (3,176)  | 1:10:A:ILE:H   | 1:35:A:PHE:HD2  | 26       | 0.26          |
| (3,176)  | 1:10:A:ILE:H   | 1:35:A:PHE:HD1  | 27       | 0.26          |
| (3,176)  | 1:10:A:ILE:H   | 1:35:A:PHE:HD2  | 27       | 0.26          |
| (3,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 29       | 0.26          |
| (3,125)  | 1:55:A:TYR:H   | 1:54:A:LYS:H    | 5        | 0.26          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 23       | 0.26          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 23       | 0.26          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 24       | 0.26          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 24       | 0.26          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 33       | 0.26          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 33       | 0.26          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 38       | 0.26          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 38       | 0.26          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 39       | 0.26          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 39       | 0.26          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 1        | 0.26          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 3        | 0.26          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 5        | 0.26          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 14       | 0.26          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 15       | 0.26          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 17       | 0.26          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 23       | 0.26          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 26       | 0.26          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 27       | 0.26          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 34       | 0.26          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 37       | 0.26          |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2 | 7        | 0.26          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2 | 7        | 0.26          |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2 | 16       | 0.26          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2 | 16       | 0.26          |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2 | 39       | 0.26          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2 | 39       | 0.26          |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2 | 40       | 0.26          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2 | 40       | 0.26          |
| (1,3048) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2 | 14       | 0.26          |
| (1,3048) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2 | 17       | 0.26          |
| (1,3048) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2 | 28       | 0.26          |
| (1,3048) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2 | 32       | 0.26          |
| (1,3048) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2 | 35       | 0.26          |
| (1,3048) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2 | 40       | 0.26          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1 | 15       | 0.26          |
| (1,2918) | 1:22:A:SER:HB2 | 1:25:A:GLN:H   | 2        | 0.26          |
| (1,2918) | 1:22:A:SER:HB2 | 1:25:A:GLN:H   | 12       | 0.26          |
| (1,2918) | 1:22:A:SER:HB2 | 1:25:A:GLN:H   | 19       | 0.26          |
| (1,2918) | 1:22:A:SER:HB2 | 1:25:A:GLN:H   | 21       | 0.26          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3  | 2        | 0.26          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3  | 9        | 0.26          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3  | 11       | 0.26          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3  | 15       | 0.26          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3  | 18       | 0.26          |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 33       | 0.26          |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 35       | 0.26          |
| (1,2467) | 1:4:A:PRO:HB2  | 1:4:A:PRO:HD2  | 5        | 0.26          |
| (1,2322) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 17       | 0.26          |
| (1,2285) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 7        | 0.26          |
| (1,2285) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 10       | 0.26          |
| (1,2285) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 11       | 0.26          |
| (1,2285) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 12       | 0.26          |
| (1,2285) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 14       | 0.26          |
| (1,2285) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 16       | 0.26          |
| (1,2285) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 17       | 0.26          |
| (1,2285) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 20       | 0.26          |
| (1,2285) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 21       | 0.26          |
| (1,2285) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 22       | 0.26          |
| (1,2285) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 24       | 0.26          |
| (1,2285) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 25       | 0.26          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2285) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H   | 26       | 0.26          |
| (1,2285) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H   | 27       | 0.26          |
| (1,2285) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H   | 30       | 0.26          |
| (1,2285) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H   | 31       | 0.26          |
| (1,2285) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H   | 32       | 0.26          |
| (1,2285) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H   | 34       | 0.26          |
| (1,2285) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H   | 35       | 0.26          |
| (1,2285) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H   | 36       | 0.26          |
| (1,2285) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H   | 38       | 0.26          |
| (1,2285) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H   | 39       | 0.26          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1 | 2        | 0.26          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2 | 2        | 0.26          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1 | 3        | 0.26          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2 | 3        | 0.26          |
| (1,2213) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 1        | 0.26          |
| (1,2213) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 3        | 0.26          |
| (1,2213) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 5        | 0.26          |
| (1,2213) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 14       | 0.26          |
| (1,2213) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 15       | 0.26          |
| (1,2213) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 17       | 0.26          |
| (1,2213) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 23       | 0.26          |
| (1,2213) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 26       | 0.26          |
| (1,2213) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 27       | 0.26          |
| (1,2213) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 34       | 0.26          |
| (1,2213) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 37       | 0.26          |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H   | 27       | 0.26          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 2        | 0.26          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 2        | 0.26          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 2        | 0.26          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 8        | 0.26          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 8        | 0.26          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 8        | 0.26          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 13       | 0.26          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 13       | 0.26          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 13       | 0.26          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 17       | 0.26          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 17       | 0.26          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 17       | 0.26          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 20       | 0.26          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 20       | 0.26          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 20       | 0.26          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 21       | 0.26          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 21       | 0.26          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 21       | 0.26          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 11       | 0.26          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 11       | 0.26          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 11       | 0.26          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 11       | 0.26          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 11       | 0.26          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 11       | 0.26          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 14       | 0.26          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 14       | 0.26          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 14       | 0.26          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 14       | 0.26          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 14       | 0.26          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 14       | 0.26          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 38       | 0.26          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 38       | 0.26          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 38       | 0.26          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 38       | 0.26          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 38       | 0.26          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 38       | 0.26          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 1        | 0.26          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 1        | 0.26          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 1        | 0.26          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 4        | 0.26          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 5        | 0.26          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 6        | 0.26          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 7        | 0.26          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 8        | 0.26          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 9        | 0.26          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 10       | 0.26          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 13       | 0.26          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 19       | 0.26          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 21       | 0.26          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 22       | 0.26          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 23       | 0.26          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 25       | 0.26          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 29       | 0.26          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 30       | 0.26          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 31       | 0.26          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 32       | 0.26          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 36       | 0.26          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 38       | 0.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 39       | 0.26          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 40       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 2        | 0.26          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 2        | 0.26          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 2        | 0.26          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 2        | 0.26          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 2        | 0.26          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 2        | 0.26          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 2        | 0.26          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 2        | 0.26          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 2        | 0.26          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 5        | 0.26          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 5        | 0.26          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 5        | 0.26          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 5        | 0.26          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 5        | 0.26          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 5        | 0.26          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 5        | 0.26          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 5        | 0.26          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 5        | 0.26          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 10       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 10       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 10       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 10       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 10       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 10       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 10       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 10       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 10       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 13       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 13       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 13       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 13       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 13       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 13       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 13       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 13       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 13       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 28       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 28       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 28       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 28       | 0.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 28       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 28       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 28       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 28       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 28       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 29       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 29       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 29       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 29       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 29       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 29       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 29       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 29       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 29       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 30       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 30       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 30       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 30       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 30       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 30       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 30       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 30       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 30       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 35       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 35       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 35       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 35       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 35       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 35       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 35       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 35       | 0.26          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 35       | 0.26          |
| (1,1778) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H    | 9        | 0.26          |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 7        | 0.26          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 7        | 0.26          |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 7        | 0.26          |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 20       | 0.26          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 20       | 0.26          |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 20       | 0.26          |
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3  | 21       | 0.26          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3  | 21       | 0.26          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3  | 21       | 0.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1669) | 1:85:A:LEU:HD21 | 1:88:A:ARG:HG3  | 24       | 0.26          |
| (1,1669) | 1:85:A:LEU:HD22 | 1:88:A:ARG:HG3  | 24       | 0.26          |
| (1,1669) | 1:85:A:LEU:HD23 | 1:88:A:ARG:HG3  | 24       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 1        | 0.26          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 1        | 0.26          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 1        | 0.26          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 2        | 0.26          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 2        | 0.26          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 2        | 0.26          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 11       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 11       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 11       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 14       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 14       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 14       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 15       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 15       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 15       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 17       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 17       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 17       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 19       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 19       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 19       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 21       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 21       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 21       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 22       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 22       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 22       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 23       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 23       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 23       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 25       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 25       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 25       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 27       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 27       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 27       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 28       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 28       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 28       | 0.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 30       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 30       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 30       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 31       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 31       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 31       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 34       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 34       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 34       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 36       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 36       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 36       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 37       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 37       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 37       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 38       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 38       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 38       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 39       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 39       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 39       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG21 | 1:10:A:ILE:HG13 | 40       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG22 | 1:10:A:ILE:HG13 | 40       | 0.26          |
| (1,1547) | 1:10:A:ILE:HG23 | 1:10:A:ILE:HG13 | 40       | 0.26          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 8        | 0.26          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 13       | 0.26          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 29       | 0.26          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 31       | 0.26          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 33       | 0.26          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 35       | 0.26          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H    | 26       | 0.26          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H    | 26       | 0.26          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H    | 26       | 0.26          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H    | 29       | 0.26          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H    | 29       | 0.26          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H    | 29       | 0.26          |
| (1,1237) | 1:13:A:THR:HG21 | 1:34:A:SER:HB2  | 6        | 0.26          |
| (1,1237) | 1:13:A:THR:HG22 | 1:34:A:SER:HB2  | 6        | 0.26          |
| (1,1237) | 1:13:A:THR:HG23 | 1:34:A:SER:HB2  | 6        | 0.26          |
| (1,1184) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 2        | 0.26          |
| (1,1184) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 5        | 0.26          |
| (1,1184) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 9        | 0.26          |

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| Key      | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|----------|--------------|-----------------|----------|---------------|
| (1,1184) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 19       | 0.26          |
| (1,1184) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 23       | 0.26          |
| (1,1184) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 25       | 0.26          |
| (1,1184) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 29       | 0.26          |
| (1,1184) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 32       | 0.26          |
| (1,1184) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 40       | 0.26          |
| (1,1163) | 1:75:A:ASP:H | 1:74:A:ASP:HB2  | 18       | 0.26          |
| (1,918)  | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 33       | 0.26          |
| (1,918)  | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 35       | 0.26          |
| (1,870)  | 1:8:A:GLU:H  | 1:9:A:PRO:HD2   | 10       | 0.26          |
| (1,849)  | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 3        | 0.26          |
| (1,849)  | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 3        | 0.26          |
| (1,849)  | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 3        | 0.26          |
| (1,685)  | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 6        | 0.26          |
| (1,685)  | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 7        | 0.26          |
| (1,685)  | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 13       | 0.26          |
| (1,685)  | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 15       | 0.26          |
| (1,685)  | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 19       | 0.26          |
| (1,685)  | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 31       | 0.26          |
| (1,685)  | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 40       | 0.26          |
| (1,584)  | 1:93:A:SER:H | 1:92:A:ARG:HB2  | 9        | 0.26          |
| (1,584)  | 1:93:A:SER:H | 1:92:A:ARG:HB2  | 12       | 0.26          |
| (1,584)  | 1:93:A:SER:H | 1:92:A:ARG:HB2  | 19       | 0.26          |
| (1,584)  | 1:93:A:SER:H | 1:92:A:ARG:HB2  | 26       | 0.26          |
| (1,546)  | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 5        | 0.26          |
| (1,546)  | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 10       | 0.26          |
| (1,525)  | 1:99:A:GLY:H | 1:100:A:GLU:H   | 14       | 0.26          |
| (1,513)  | 1:67:A:THR:H | 1:66:A:MET:HG3  | 10       | 0.26          |
| (1,513)  | 1:67:A:THR:H | 1:66:A:MET:HG3  | 19       | 0.26          |
| (1,423)  | 1:69:A:HIS:H | 1:69:A:HIS:HD2  | 6        | 0.26          |
| (1,423)  | 1:69:A:HIS:H | 1:69:A:HIS:HD2  | 16       | 0.26          |
| (1,423)  | 1:69:A:HIS:H | 1:69:A:HIS:HD2  | 18       | 0.26          |
| (1,343)  | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 3        | 0.26          |
| (1,343)  | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 17       | 0.26          |
| (1,343)  | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 27       | 0.26          |
| (1,176)  | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 26       | 0.26          |
| (1,176)  | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 26       | 0.26          |
| (1,176)  | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 27       | 0.26          |
| (1,176)  | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 27       | 0.26          |
| (1,169)  | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 29       | 0.26          |
| (1,149)  | 1:45:A:GLY:H | 1:46:A:PRO:HD3  | 1        | 0.26          |
| (1,149)  | 1:45:A:GLY:H | 1:46:A:PRO:HD3  | 7        | 0.26          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,123)  | 1:55:A:TYR:H   | 1:54:A:LYS:H   | 5        | 0.26          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3 | 8        | 0.25          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3 | 8        | 0.25          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 4        | 0.25          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 8        | 0.25          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 9        | 0.25          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 10       | 0.25          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 11       | 0.25          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 16       | 0.25          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 18       | 0.25          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 20       | 0.25          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 22       | 0.25          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 24       | 0.25          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 25       | 0.25          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 28       | 0.25          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 30       | 0.25          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 31       | 0.25          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 32       | 0.25          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 33       | 0.25          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 35       | 0.25          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3 | 36       | 0.25          |
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2 | 3        | 0.25          |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2 | 3        | 0.25          |
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2 | 6        | 0.25          |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2 | 6        | 0.25          |
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2 | 14       | 0.25          |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2 | 14       | 0.25          |
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2 | 28       | 0.25          |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2 | 28       | 0.25          |
| (3,3056) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2 | 1        | 0.25          |
| (3,3056) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2 | 15       | 0.25          |
| (3,3056) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2 | 22       | 0.25          |
| (3,3056) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2 | 36       | 0.25          |
| (3,3056) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2 | 39       | 0.25          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1 | 10       | 0.25          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1 | 21       | 0.25          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1 | 30       | 0.25          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1 | 33       | 0.25          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1 | 39       | 0.25          |
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 1        | 0.25          |
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 9        | 0.25          |
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 13       | 0.25          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H    | 15       | 0.25          |
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H    | 18       | 0.25          |
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H    | 22       | 0.25          |
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H    | 23       | 0.25          |
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H    | 30       | 0.25          |
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H    | 38       | 0.25          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 17       | 0.25          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 17       | 0.25          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 17       | 0.25          |
| (3,2925) | 1:22:A:SER:HB2 | 1:25:A:GLN:H    | 25       | 0.25          |
| (3,2925) | 1:22:A:SER:HB2 | 1:25:A:GLN:H    | 38       | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 1        | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 2        | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 3        | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 4        | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 5        | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 6        | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 7        | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 10       | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 11       | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 13       | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 14       | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 16       | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 17       | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 18       | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 19       | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 21       | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 22       | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 23       | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 24       | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 25       | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 26       | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 27       | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 30       | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 31       | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 32       | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 33       | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 34       | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 36       | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 37       | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 38       | 0.25          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 39       | 0.25          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3 | 40       | 0.25          |
| (3,2722) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 20       | 0.25          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 7        | 0.25          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 18       | 0.25          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 31       | 0.25          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 39       | 0.25          |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 4        | 0.25          |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 34       | 0.25          |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 37       | 0.25          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 26       | 0.25          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 27       | 0.25          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 28       | 0.25          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 30       | 0.25          |
| (3,2485) | 1:9:A:PRO:HD3  | 1:9:A:PRO:HB3  | 26       | 0.25          |
| (3,2485) | 1:9:A:PRO:HD3  | 1:9:A:PRO:HB3  | 27       | 0.25          |
| (3,2485) | 1:9:A:PRO:HD3  | 1:9:A:PRO:HB3  | 29       | 0.25          |
| (3,2485) | 1:9:A:PRO:HD3  | 1:9:A:PRO:HB3  | 37       | 0.25          |
| (3,2485) | 1:9:A:PRO:HD3  | 1:9:A:PRO:HB3  | 40       | 0.25          |
| (3,2470) | 1:4:A:PRO:HB2  | 1:4:A:PRO:HD2  | 8        | 0.25          |
| (3,2470) | 1:4:A:PRO:HB2  | 1:4:A:PRO:HD2  | 11       | 0.25          |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 15       | 0.25          |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 38       | 0.25          |
| (3,2288) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 2        | 0.25          |
| (3,2288) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 4        | 0.25          |
| (3,2288) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 18       | 0.25          |
| (3,2288) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 19       | 0.25          |
| (3,2288) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 28       | 0.25          |
| (3,2216) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 4        | 0.25          |
| (3,2216) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 8        | 0.25          |
| (3,2216) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 9        | 0.25          |
| (3,2216) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 10       | 0.25          |
| (3,2216) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 11       | 0.25          |
| (3,2216) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 16       | 0.25          |
| (3,2216) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 18       | 0.25          |
| (3,2216) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 20       | 0.25          |
| (3,2216) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 22       | 0.25          |
| (3,2216) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 24       | 0.25          |
| (3,2216) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 25       | 0.25          |
| (3,2216) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 28       | 0.25          |
| (3,2216) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 30       | 0.25          |
| (3,2216) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 31       | 0.25          |
| (3,2216) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 32       | 0.25          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2216) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 33       | 0.25          |
| (3,2216) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 35       | 0.25          |
| (3,2216) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 36       | 0.25          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 12       | 0.25          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 12       | 0.25          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 12       | 0.25          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 22       | 0.25          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 22       | 0.25          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 22       | 0.25          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 24       | 0.25          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 24       | 0.25          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 24       | 0.25          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 31       | 0.25          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 31       | 0.25          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 31       | 0.25          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 39       | 0.25          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 39       | 0.25          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 39       | 0.25          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 40       | 0.25          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 40       | 0.25          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 40       | 0.25          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 3        | 0.25          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 3        | 0.25          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 3        | 0.25          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 3        | 0.25          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 3        | 0.25          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 3        | 0.25          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 20       | 0.25          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 20       | 0.25          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 20       | 0.25          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 20       | 0.25          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 20       | 0.25          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 20       | 0.25          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 26       | 0.25          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 26       | 0.25          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 26       | 0.25          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 26       | 0.25          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 26       | 0.25          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 26       | 0.25          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 34       | 0.25          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 34       | 0.25          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 34       | 0.25          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 34       | 0.25          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 34       | 0.25          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 34       | 0.25          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 28       | 0.25          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 28       | 0.25          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 28       | 0.25          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 22       | 0.25          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 22       | 0.25          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 22       | 0.25          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 23       | 0.25          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 23       | 0.25          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 23       | 0.25          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 31       | 0.25          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 31       | 0.25          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 31       | 0.25          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 1        | 0.25          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 9        | 0.25          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 12       | 0.25          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 2        | 0.25          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 3        | 0.25          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 11       | 0.25          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 12       | 0.25          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 14       | 0.25          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 16       | 0.25          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 17       | 0.25          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 20       | 0.25          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 24       | 0.25          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 26       | 0.25          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 28       | 0.25          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 33       | 0.25          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 34       | 0.25          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 35       | 0.25          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 37       | 0.25          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 33       | 0.25          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 33       | 0.25          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 33       | 0.25          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 1        | 0.25          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 9        | 0.25          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 12       | 0.25          |
| (3,1781) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H   | 10       | 0.25          |
| (3,1781) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H   | 17       | 0.25          |
| (3,1696) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H   | 15       | 0.25          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1696) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 15       | 0.25          |
| (3,1696) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 15       | 0.25          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 10       | 0.25          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 10       | 0.25          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 10       | 0.25          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 10       | 0.25          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 10       | 0.25          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 10       | 0.25          |
| (3,1540) | 1:39:A:ILE:HD11 | 1:40:A:VAL:H    | 11       | 0.25          |
| (3,1540) | 1:39:A:ILE:HD12 | 1:40:A:VAL:H    | 11       | 0.25          |
| (3,1540) | 1:39:A:ILE:HD13 | 1:40:A:VAL:H    | 11       | 0.25          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 1        | 0.25          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 12       | 0.25          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 15       | 0.25          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 18       | 0.25          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 19       | 0.25          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 21       | 0.25          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 22       | 0.25          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 32       | 0.25          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 34       | 0.25          |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3  | 8        | 0.25          |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3  | 8        | 0.25          |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3  | 8        | 0.25          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H    | 39       | 0.25          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H    | 39       | 0.25          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H    | 39       | 0.25          |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 11       | 0.25          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 14       | 0.25          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 14       | 0.25          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 14       | 0.25          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 6        | 0.25          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 6        | 0.25          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 6        | 0.25          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 16       | 0.25          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 16       | 0.25          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 16       | 0.25          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 4        | 0.25          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 4        | 0.25          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 4        | 0.25          |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 21       | 0.25          |
| (3,1188) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 4        | 0.25          |
| (3,1188) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 12       | 0.25          |

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| Key      | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|----------|--------------|-----------------|----------|---------------|
| (3,1188) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 26       | 0.25          |
| (3,1188) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 27       | 0.25          |
| (3,1188) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 38       | 0.25          |
| (3,935)  | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 15       | 0.25          |
| (3,935)  | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 15       | 0.25          |
| (3,935)  | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 15       | 0.25          |
| (3,919)  | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 4        | 0.25          |
| (3,919)  | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 34       | 0.25          |
| (3,919)  | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 37       | 0.25          |
| (3,871)  | 1:8:A:GLU:H  | 1:9:A:PRO:HD3   | 30       | 0.25          |
| (3,869)  | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 4        | 0.25          |
| (3,869)  | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 26       | 0.25          |
| (3,849)  | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 9        | 0.25          |
| (3,849)  | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 9        | 0.25          |
| (3,849)  | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 9        | 0.25          |
| (3,826)  | 1:17:A:GLN:H | 1:17:A:GLN:HG2  | 5        | 0.25          |
| (3,826)  | 1:17:A:GLN:H | 1:17:A:GLN:HG2  | 26       | 0.25          |
| (3,814)  | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 20       | 0.25          |
| (3,814)  | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 20       | 0.25          |
| (3,814)  | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 20       | 0.25          |
| (3,814)  | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 26       | 0.25          |
| (3,814)  | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 26       | 0.25          |
| (3,814)  | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 26       | 0.25          |
| (3,768)  | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 1        | 0.25          |
| (3,768)  | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 2        | 0.25          |
| (3,768)  | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 3        | 0.25          |
| (3,768)  | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 4        | 0.25          |
| (3,768)  | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 5        | 0.25          |
| (3,768)  | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 6        | 0.25          |
| (3,768)  | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 7        | 0.25          |
| (3,768)  | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 9        | 0.25          |
| (3,768)  | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 10       | 0.25          |
| (3,768)  | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 11       | 0.25          |
| (3,768)  | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 13       | 0.25          |
| (3,768)  | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 17       | 0.25          |
| (3,768)  | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 18       | 0.25          |
| (3,768)  | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 19       | 0.25          |
| (3,768)  | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 37       | 0.25          |
| (3,715)  | 1:16:A:ILE:H | 1:15:A:ARG:HB3  | 27       | 0.25          |
| (3,685)  | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 10       | 0.25          |
| (3,685)  | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 11       | 0.25          |
| (3,685)  | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 12       | 0.25          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 14       | 0.25          |
| (3,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 16       | 0.25          |
| (3,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 17       | 0.25          |
| (3,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 32       | 0.25          |
| (3,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 36       | 0.25          |
| (3,584) | 1:93:A:SER:H | 1:92:A:ARG:HB2  | 16       | 0.25          |
| (3,584) | 1:93:A:SER:H | 1:92:A:ARG:HB2  | 29       | 0.25          |
| (3,584) | 1:93:A:SER:H | 1:92:A:ARG:HB2  | 33       | 0.25          |
| (3,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 22       | 0.25          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 2        | 0.25          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 4        | 0.25          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 24       | 0.25          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 33       | 0.25          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 40       | 0.25          |
| (3,513) | 1:67:A:THR:H | 1:66:A:MET:HG3  | 7        | 0.25          |
| (3,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2  | 13       | 0.25          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3  | 2        | 0.25          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3  | 7        | 0.25          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3  | 22       | 0.25          |
| (3,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 5        | 0.25          |
| (3,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 21       | 0.25          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 4        | 0.25          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 4        | 0.25          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 13       | 0.25          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 13       | 0.25          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 17       | 0.25          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 17       | 0.25          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 20       | 0.25          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 20       | 0.25          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 30       | 0.25          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 30       | 0.25          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 36       | 0.25          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 36       | 0.25          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 2        | 0.25          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 12       | 0.25          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 13       | 0.25          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 16       | 0.25          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 22       | 0.25          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 23       | 0.25          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 31       | 0.25          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 34       | 0.25          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 36       | 0.25          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 38       | 0.25          |
| (3,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 39       | 0.25          |
| (3,125)  | 1:55:A:TYR:H   | 1:54:A:LYS:H    | 7        | 0.25          |
| (3,22)   | 1:89:A:GLY:H   | 1:85:A:LEU:H    | 26       | 0.25          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 8        | 0.25          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 8        | 0.25          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 4        | 0.25          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 8        | 0.25          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 9        | 0.25          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 10       | 0.25          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 11       | 0.25          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 16       | 0.25          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 18       | 0.25          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 20       | 0.25          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 22       | 0.25          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 24       | 0.25          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 25       | 0.25          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 28       | 0.25          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 30       | 0.25          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 31       | 0.25          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 32       | 0.25          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 33       | 0.25          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 35       | 0.25          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 36       | 0.25          |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 3        | 0.25          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 3        | 0.25          |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 6        | 0.25          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 6        | 0.25          |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 14       | 0.25          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 14       | 0.25          |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 28       | 0.25          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 28       | 0.25          |
| (1,3048) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2  | 1        | 0.25          |
| (1,3048) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2  | 15       | 0.25          |
| (1,3048) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2  | 22       | 0.25          |
| (1,3048) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2  | 36       | 0.25          |
| (1,3048) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2  | 39       | 0.25          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 10       | 0.25          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 21       | 0.25          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 30       | 0.25          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 33       | 0.25          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 39       | 0.25          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H    | 1        | 0.25          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H    | 9        | 0.25          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H    | 13       | 0.25          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H    | 15       | 0.25          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H    | 18       | 0.25          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H    | 22       | 0.25          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H    | 23       | 0.25          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H    | 30       | 0.25          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H    | 38       | 0.25          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 17       | 0.25          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 17       | 0.25          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 17       | 0.25          |
| (1,2918) | 1:22:A:SER:HB2 | 1:25:A:GLN:H    | 25       | 0.25          |
| (1,2918) | 1:22:A:SER:HB2 | 1:25:A:GLN:H    | 38       | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 1        | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 2        | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 3        | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 4        | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 5        | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 6        | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 7        | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 10       | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 11       | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 13       | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 14       | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 16       | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 17       | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 18       | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 19       | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 21       | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 22       | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 23       | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 24       | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 25       | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 26       | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 27       | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 30       | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 31       | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 32       | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 33       | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 34       | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3  | 36       | 0.25          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3 | 37       | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3 | 38       | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3 | 39       | 0.25          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3 | 40       | 0.25          |
| (1,2718) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 20       | 0.25          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 7        | 0.25          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 18       | 0.25          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 31       | 0.25          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 39       | 0.25          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3  | 10       | 0.25          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3  | 12       | 0.25          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3  | 13       | 0.25          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3  | 16       | 0.25          |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 4        | 0.25          |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 34       | 0.25          |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 37       | 0.25          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 26       | 0.25          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 27       | 0.25          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 28       | 0.25          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 30       | 0.25          |
| (1,2467) | 1:4:A:PRO:HB2  | 1:4:A:PRO:HD2  | 8        | 0.25          |
| (1,2467) | 1:4:A:PRO:HB2  | 1:4:A:PRO:HD2  | 11       | 0.25          |
| (1,2322) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 15       | 0.25          |
| (1,2322) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 38       | 0.25          |
| (1,2285) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 2        | 0.25          |
| (1,2285) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 4        | 0.25          |
| (1,2285) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 18       | 0.25          |
| (1,2285) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 19       | 0.25          |
| (1,2285) | 1:96:A:GLU:HG3 | 1:97:A:LEU:H   | 28       | 0.25          |
| (1,2213) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 4        | 0.25          |
| (1,2213) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 8        | 0.25          |
| (1,2213) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 9        | 0.25          |
| (1,2213) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 10       | 0.25          |
| (1,2213) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 11       | 0.25          |
| (1,2213) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 16       | 0.25          |
| (1,2213) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 18       | 0.25          |
| (1,2213) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 20       | 0.25          |
| (1,2213) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 22       | 0.25          |
| (1,2213) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 24       | 0.25          |
| (1,2213) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 25       | 0.25          |
| (1,2213) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 28       | 0.25          |
| (1,2213) | 1:42:A:TRP:HB3 | 1:42:A:TRP:HD1 | 30       | 0.25          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2213) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 31       | 0.25          |
| (1,2213) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 32       | 0.25          |
| (1,2213) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 33       | 0.25          |
| (1,2213) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 35       | 0.25          |
| (1,2213) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 36       | 0.25          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 12       | 0.25          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 12       | 0.25          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 12       | 0.25          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 22       | 0.25          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 22       | 0.25          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 22       | 0.25          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 24       | 0.25          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 24       | 0.25          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 24       | 0.25          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 31       | 0.25          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 31       | 0.25          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 31       | 0.25          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 39       | 0.25          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 39       | 0.25          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 39       | 0.25          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 40       | 0.25          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 40       | 0.25          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 40       | 0.25          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 3        | 0.25          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 3        | 0.25          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 3        | 0.25          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 3        | 0.25          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 3        | 0.25          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 3        | 0.25          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 20       | 0.25          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 20       | 0.25          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 20       | 0.25          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 20       | 0.25          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 20       | 0.25          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 20       | 0.25          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 26       | 0.25          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 26       | 0.25          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 26       | 0.25          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 26       | 0.25          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 26       | 0.25          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 26       | 0.25          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 34       | 0.25          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2  | 34       | 0.25          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1  | 34       | 0.25          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2  | 34       | 0.25          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1  | 34       | 0.25          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2  | 34       | 0.25          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 28       | 0.25          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 28       | 0.25          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 28       | 0.25          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3  | 22       | 0.25          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3  | 22       | 0.25          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3  | 22       | 0.25          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3  | 23       | 0.25          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3  | 23       | 0.25          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3  | 23       | 0.25          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3  | 31       | 0.25          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3  | 31       | 0.25          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3  | 31       | 0.25          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2  | 1        | 0.25          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2  | 9        | 0.25          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2  | 12       | 0.25          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 2        | 0.25          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 3        | 0.25          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 11       | 0.25          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 12       | 0.25          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 14       | 0.25          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 16       | 0.25          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 17       | 0.25          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 20       | 0.25          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 24       | 0.25          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 26       | 0.25          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 28       | 0.25          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 33       | 0.25          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 34       | 0.25          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 35       | 0.25          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3  | 37       | 0.25          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA   | 33       | 0.25          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA   | 33       | 0.25          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA   | 33       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 15       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 15       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 15       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 15       | 0.25          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 15       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 15       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 15       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 15       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 15       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 17       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 17       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 17       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 17       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 17       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 17       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 17       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 17       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 17       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 24       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 24       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 24       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 24       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 24       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 24       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 24       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 24       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 24       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 32       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 32       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 32       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 32       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 32       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 32       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 32       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 32       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 32       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 37       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 37       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 37       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 37       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 37       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 37       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 37       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 37       | 0.25          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 37       | 0.25          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2  | 1        | 0.25          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2  | 9        | 0.25          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2  | 12       | 0.25          |
| (1,1778) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H    | 10       | 0.25          |
| (1,1778) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H    | 17       | 0.25          |
| (1,1692) | 1:97:A:LEU:HD21 | 1:98:A:LYS:H    | 15       | 0.25          |
| (1,1692) | 1:97:A:LEU:HD22 | 1:98:A:LYS:H    | 15       | 0.25          |
| (1,1692) | 1:97:A:LEU:HD23 | 1:98:A:LYS:H    | 15       | 0.25          |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 10       | 0.25          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 10       | 0.25          |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 10       | 0.25          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 10       | 0.25          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 10       | 0.25          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 10       | 0.25          |
| (1,1536) | 1:39:A:ILE:HD11 | 1:40:A:VAL:H    | 11       | 0.25          |
| (1,1536) | 1:39:A:ILE:HD12 | 1:40:A:VAL:H    | 11       | 0.25          |
| (1,1536) | 1:39:A:ILE:HD13 | 1:40:A:VAL:H    | 11       | 0.25          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 1        | 0.25          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 12       | 0.25          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 15       | 0.25          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 18       | 0.25          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 19       | 0.25          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 21       | 0.25          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 22       | 0.25          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 32       | 0.25          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 34       | 0.25          |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3  | 8        | 0.25          |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3  | 8        | 0.25          |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3  | 8        | 0.25          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H    | 39       | 0.25          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H    | 39       | 0.25          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H    | 39       | 0.25          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 11       | 0.25          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 14       | 0.25          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 14       | 0.25          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 14       | 0.25          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 6        | 0.25          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 6        | 0.25          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 6        | 0.25          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 16       | 0.25          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 16       | 0.25          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 16       | 0.25          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 4        | 0.25          |

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| Key      | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|----------|--------------|-----------------|----------|---------------|
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 4        | 0.25          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 4        | 0.25          |
| (1,1185) | 1:21:A:VAL:H | 1:100:A:GLU:HB3 | 21       | 0.25          |
| (1,1184) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 4        | 0.25          |
| (1,1184) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 12       | 0.25          |
| (1,1184) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 26       | 0.25          |
| (1,1184) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 27       | 0.25          |
| (1,1184) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 38       | 0.25          |
| (1,934)  | 1:98:A:LYS:H | 1:97:A:LEU:HD21 | 15       | 0.25          |
| (1,934)  | 1:98:A:LYS:H | 1:97:A:LEU:HD22 | 15       | 0.25          |
| (1,934)  | 1:98:A:LYS:H | 1:97:A:LEU:HD23 | 15       | 0.25          |
| (1,918)  | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 4        | 0.25          |
| (1,918)  | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 34       | 0.25          |
| (1,918)  | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 37       | 0.25          |
| (1,871)  | 1:8:A:GLU:H  | 1:9:A:PRO:HD3   | 30       | 0.25          |
| (1,869)  | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 4        | 0.25          |
| (1,869)  | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 26       | 0.25          |
| (1,849)  | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 9        | 0.25          |
| (1,849)  | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 9        | 0.25          |
| (1,849)  | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 9        | 0.25          |
| (1,826)  | 1:17:A:GLN:H | 1:17:A:GLN:HG2  | 5        | 0.25          |
| (1,826)  | 1:17:A:GLN:H | 1:17:A:GLN:HG2  | 26       | 0.25          |
| (1,814)  | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 20       | 0.25          |
| (1,814)  | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 20       | 0.25          |
| (1,814)  | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 20       | 0.25          |
| (1,814)  | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 26       | 0.25          |
| (1,814)  | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 26       | 0.25          |
| (1,814)  | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 26       | 0.25          |
| (1,768)  | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 1        | 0.25          |
| (1,768)  | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 2        | 0.25          |
| (1,768)  | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 3        | 0.25          |
| (1,768)  | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 4        | 0.25          |
| (1,768)  | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 5        | 0.25          |
| (1,768)  | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 6        | 0.25          |
| (1,768)  | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 7        | 0.25          |
| (1,768)  | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 9        | 0.25          |
| (1,768)  | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 10       | 0.25          |
| (1,768)  | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 11       | 0.25          |
| (1,768)  | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 13       | 0.25          |
| (1,768)  | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 17       | 0.25          |
| (1,768)  | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 18       | 0.25          |
| (1,768)  | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 19       | 0.25          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 37       | 0.25          |
| (1,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3  | 27       | 0.25          |
| (1,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 10       | 0.25          |
| (1,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 11       | 0.25          |
| (1,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 12       | 0.25          |
| (1,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 14       | 0.25          |
| (1,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 16       | 0.25          |
| (1,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 17       | 0.25          |
| (1,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 32       | 0.25          |
| (1,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 36       | 0.25          |
| (1,584) | 1:93:A:SER:H | 1:92:A:ARG:HB2  | 16       | 0.25          |
| (1,584) | 1:93:A:SER:H | 1:92:A:ARG:HB2  | 29       | 0.25          |
| (1,584) | 1:93:A:SER:H | 1:92:A:ARG:HB2  | 33       | 0.25          |
| (1,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 22       | 0.25          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 2        | 0.25          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 4        | 0.25          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 24       | 0.25          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 33       | 0.25          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 40       | 0.25          |
| (1,513) | 1:67:A:THR:H | 1:66:A:MET:HG3  | 7        | 0.25          |
| (1,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2  | 13       | 0.25          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3  | 2        | 0.25          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3  | 7        | 0.25          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3  | 22       | 0.25          |
| (1,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 5        | 0.25          |
| (1,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 21       | 0.25          |
| (1,199) | 1:90:A:GLU:H | 1:10:A:ILE:HG21 | 33       | 0.25          |
| (1,199) | 1:90:A:GLU:H | 1:10:A:ILE:HG22 | 33       | 0.25          |
| (1,199) | 1:90:A:GLU:H | 1:10:A:ILE:HG23 | 33       | 0.25          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 4        | 0.25          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 4        | 0.25          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 13       | 0.25          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 13       | 0.25          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 17       | 0.25          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 17       | 0.25          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 20       | 0.25          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 20       | 0.25          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 30       | 0.25          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 30       | 0.25          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 36       | 0.25          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 36       | 0.25          |
| (1,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 2        | 0.25          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 12       | 0.25          |
| (1,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 13       | 0.25          |
| (1,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 16       | 0.25          |
| (1,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 22       | 0.25          |
| (1,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 23       | 0.25          |
| (1,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 31       | 0.25          |
| (1,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 34       | 0.25          |
| (1,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 36       | 0.25          |
| (1,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 38       | 0.25          |
| (1,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 39       | 0.25          |
| (1,123)  | 1:55:A:TYR:H   | 1:54:A:LYS:H    | 7        | 0.25          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 5        | 0.24          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 5        | 0.24          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 16       | 0.24          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 16       | 0.24          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 18       | 0.24          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 18       | 0.24          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 20       | 0.24          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 20       | 0.24          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 30       | 0.24          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 30       | 0.24          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 37       | 0.24          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 37       | 0.24          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 5        | 0.24          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 14       | 0.24          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 2        | 0.24          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 6        | 0.24          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 7        | 0.24          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 12       | 0.24          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 19       | 0.24          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 21       | 0.24          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 29       | 0.24          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 39       | 0.24          |
| (3,3165) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 40       | 0.24          |
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 8        | 0.24          |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 8        | 0.24          |
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 9        | 0.24          |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 9        | 0.24          |
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 12       | 0.24          |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 12       | 0.24          |
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 24       | 0.24          |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 24       | 0.24          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2 | 26       | 0.24          |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2 | 26       | 0.24          |
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2 | 27       | 0.24          |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2 | 27       | 0.24          |
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2 | 38       | 0.24          |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2 | 38       | 0.24          |
| (3,3056) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2 | 7        | 0.24          |
| (3,3056) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2 | 18       | 0.24          |
| (3,3056) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2 | 25       | 0.24          |
| (3,3056) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2 | 34       | 0.24          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1 | 2        | 0.24          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1 | 6        | 0.24          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1 | 17       | 0.24          |
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 2        | 0.24          |
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 3        | 0.24          |
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 5        | 0.24          |
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 8        | 0.24          |
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 10       | 0.24          |
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 11       | 0.24          |
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 12       | 0.24          |
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 14       | 0.24          |
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 16       | 0.24          |
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 20       | 0.24          |
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 21       | 0.24          |
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 24       | 0.24          |
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 25       | 0.24          |
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 26       | 0.24          |
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 27       | 0.24          |
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 29       | 0.24          |
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 31       | 0.24          |
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 32       | 0.24          |
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 33       | 0.24          |
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 37       | 0.24          |
| (3,3054) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 40       | 0.24          |
| (3,2925) | 1:22:A:SER:HB2 | 1:25:A:GLN:H   | 8        | 0.24          |
| (3,2925) | 1:22:A:SER:HB2 | 1:25:A:GLN:H   | 17       | 0.24          |
| (3,2925) | 1:22:A:SER:HB2 | 1:25:A:GLN:H   | 22       | 0.24          |
| (3,2925) | 1:22:A:SER:HB2 | 1:25:A:GLN:H   | 23       | 0.24          |
| (3,2925) | 1:22:A:SER:HB2 | 1:25:A:GLN:H   | 24       | 0.24          |
| (3,2925) | 1:22:A:SER:HB2 | 1:25:A:GLN:H   | 26       | 0.24          |
| (3,2925) | 1:22:A:SER:HB2 | 1:25:A:GLN:H   | 30       | 0.24          |
| (3,2923) | 1:22:A:SER:HB2 | 1:22:A:SER:H   | 6        | 0.24          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3 | 8        | 0.24          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3 | 9        | 0.24          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3 | 12       | 0.24          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3 | 15       | 0.24          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3 | 20       | 0.24          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3 | 28       | 0.24          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3 | 29       | 0.24          |
| (3,2746) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3 | 35       | 0.24          |
| (3,2722) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 13       | 0.24          |
| (3,2722) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 14       | 0.24          |
| (3,2722) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 15       | 0.24          |
| (3,2722) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 22       | 0.24          |
| (3,2722) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 26       | 0.24          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 6        | 0.24          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 8        | 0.24          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 12       | 0.24          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 13       | 0.24          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 19       | 0.24          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 28       | 0.24          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 29       | 0.24          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 33       | 0.24          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 35       | 0.24          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 36       | 0.24          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 40       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 1        | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 2        | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 3        | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 4        | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 5        | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 6        | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 7        | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 8        | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 9        | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 10       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 11       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 12       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 13       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 14       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 15       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 16       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 17       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 18       | 0.24          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 19       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 20       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 21       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 22       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 23       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 24       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 25       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 26       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 27       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 28       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 29       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 30       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 31       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 32       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 33       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 34       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 35       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 36       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 37       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 38       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 39       | 0.24          |
| (3,2671) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 40       | 0.24          |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 5        | 0.24          |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 30       | 0.24          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 21       | 0.24          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 22       | 0.24          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 24       | 0.24          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 25       | 0.24          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 29       | 0.24          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 32       | 0.24          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 33       | 0.24          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 34       | 0.24          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 35       | 0.24          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 38       | 0.24          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 39       | 0.24          |
| (3,2538) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 18       | 0.24          |
| (3,2515) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD3 | 11       | 0.24          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 28       | 0.24          |
| (3,2485) | 1:9:A:PRO:HD3  | 1:9:A:PRO:HB3  | 28       | 0.24          |
| (3,2485) | 1:9:A:PRO:HD3  | 1:9:A:PRO:HB3  | 30       | 0.24          |
| (3,2485) | 1:9:A:PRO:HD3  | 1:9:A:PRO:HB3  | 31       | 0.24          |
| (3,2485) | 1:9:A:PRO:HD3  | 1:9:A:PRO:HB3  | 34       | 0.24          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2485) | 1:9:A:PRO:HD3   | 1:9:A:PRO:HB3  | 38       | 0.24          |
| (3,2482) | 1:9:A:PRO:HD2   | 1:8:A:GLU:HA   | 16       | 0.24          |
| (3,2470) | 1:4:A:PRO:HB2   | 1:4:A:PRO:HD2  | 15       | 0.24          |
| (3,2434) | 1:82:A:ILE:HB   | 1:41:A:THR:H   | 17       | 0.24          |
| (3,2434) | 1:82:A:ILE:HB   | 1:41:A:THR:H   | 34       | 0.24          |
| (3,2325) | 1:80:A:SER:HB2  | 1:81:A:VAL:H   | 6        | 0.24          |
| (3,2325) | 1:80:A:SER:HB2  | 1:81:A:VAL:H   | 14       | 0.24          |
| (3,2325) | 1:80:A:SER:HB2  | 1:81:A:VAL:H   | 39       | 0.24          |
| (3,2288) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H   | 3        | 0.24          |
| (3,2288) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H   | 5        | 0.24          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1 | 1        | 0.24          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2 | 1        | 0.24          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1 | 19       | 0.24          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2 | 19       | 0.24          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1 | 28       | 0.24          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2 | 28       | 0.24          |
| (3,2216) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 2        | 0.24          |
| (3,2216) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 6        | 0.24          |
| (3,2216) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 7        | 0.24          |
| (3,2216) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 12       | 0.24          |
| (3,2216) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 19       | 0.24          |
| (3,2216) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 21       | 0.24          |
| (3,2216) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 29       | 0.24          |
| (3,2216) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 39       | 0.24          |
| (3,2216) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 40       | 0.24          |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H   | 20       | 0.24          |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H   | 21       | 0.24          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 3        | 0.24          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 3        | 0.24          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 3        | 0.24          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 4        | 0.24          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 4        | 0.24          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 4        | 0.24          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 6        | 0.24          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 6        | 0.24          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 6        | 0.24          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 7        | 0.24          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 7        | 0.24          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 7        | 0.24          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 10       | 0.24          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 10       | 0.24          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 10       | 0.24          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 11       | 0.24          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 11       | 0.24          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 11       | 0.24          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 16       | 0.24          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 16       | 0.24          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 16       | 0.24          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 32       | 0.24          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 32       | 0.24          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 32       | 0.24          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 34       | 0.24          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 34       | 0.24          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 34       | 0.24          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 36       | 0.24          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 36       | 0.24          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 36       | 0.24          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 38       | 0.24          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 38       | 0.24          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 38       | 0.24          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 5        | 0.24          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 5        | 0.24          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 5        | 0.24          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 5        | 0.24          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 5        | 0.24          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 5        | 0.24          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 23       | 0.24          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 23       | 0.24          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 23       | 0.24          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 23       | 0.24          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 23       | 0.24          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 23       | 0.24          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 25       | 0.24          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 25       | 0.24          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 25       | 0.24          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 25       | 0.24          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 25       | 0.24          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 25       | 0.24          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 5        | 0.24          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 5        | 0.24          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 5        | 0.24          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 7        | 0.24          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 7        | 0.24          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 7        | 0.24          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 26       | 0.24          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 26       | 0.24          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 26       | 0.24          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 32       | 0.24          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 32       | 0.24          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 32       | 0.24          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 3        | 0.24          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 4        | 0.24          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 5        | 0.24          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 7        | 0.24          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 10       | 0.24          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 13       | 0.24          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 14       | 0.24          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 15       | 0.24          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 17       | 0.24          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 19       | 0.24          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 20       | 0.24          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 21       | 0.24          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 22       | 0.24          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 23       | 0.24          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 24       | 0.24          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 25       | 0.24          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 29       | 0.24          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 30       | 0.24          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 31       | 0.24          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 32       | 0.24          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 34       | 0.24          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 35       | 0.24          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 36       | 0.24          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 38       | 0.24          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 39       | 0.24          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 40       | 0.24          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 15       | 0.24          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 18       | 0.24          |
| (3,1962) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 27       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 2        | 0.24          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 2        | 0.24          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 2        | 0.24          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 3        | 0.24          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 3        | 0.24          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 3        | 0.24          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 4        | 0.24          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA | 4        | 0.24          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA | 4        | 0.24          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA | 7        | 0.24          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA | 7        | 0.24          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA | 7        | 0.24          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA | 10       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA | 10       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA | 10       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA | 11       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA | 11       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA | 11       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA | 12       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA | 12       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA | 12       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA | 16       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA | 16       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA | 16       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA | 18       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA | 18       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA | 18       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA | 19       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA | 19       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA | 19       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA | 21       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA | 21       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA | 21       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA | 22       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA | 22       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA | 22       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA | 24       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA | 24       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA | 24       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA | 26       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA | 26       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA | 26       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA | 28       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA | 28       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA | 28       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA | 29       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA | 29       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA | 29       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA | 31       | 0.24          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 31       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 31       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 32       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 32       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 32       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 36       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 36       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 36       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 37       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 37       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 37       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 38       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 38       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 38       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 39       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 39       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 39       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 40       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 40       | 0.24          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 40       | 0.24          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 1        | 0.24          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 7        | 0.24          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 16       | 0.24          |
| (3,1907) | 1:66:A:MET:HE1  | 1:43:A:TYR:H   | 12       | 0.24          |
| (3,1907) | 1:66:A:MET:HE2  | 1:43:A:TYR:H   | 12       | 0.24          |
| (3,1907) | 1:66:A:MET:HE3  | 1:43:A:TYR:H   | 12       | 0.24          |
| (3,1907) | 1:66:A:MET:HE1  | 1:43:A:TYR:H   | 19       | 0.24          |
| (3,1907) | 1:66:A:MET:HE2  | 1:43:A:TYR:H   | 19       | 0.24          |
| (3,1907) | 1:66:A:MET:HE3  | 1:43:A:TYR:H   | 19       | 0.24          |
| (3,1907) | 1:66:A:MET:HE1  | 1:43:A:TYR:H   | 39       | 0.24          |
| (3,1907) | 1:66:A:MET:HE2  | 1:43:A:TYR:H   | 39       | 0.24          |
| (3,1907) | 1:66:A:MET:HE3  | 1:43:A:TYR:H   | 39       | 0.24          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 3        | 0.24          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 4        | 0.24          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 5        | 0.24          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 7        | 0.24          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 10       | 0.24          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 13       | 0.24          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 14       | 0.24          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 15       | 0.24          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 17       | 0.24          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 19       | 0.24          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 20       | 0.24          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 21       | 0.24          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 22       | 0.24          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 23       | 0.24          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 24       | 0.24          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 25       | 0.24          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 29       | 0.24          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 30       | 0.24          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 31       | 0.24          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 32       | 0.24          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 34       | 0.24          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 35       | 0.24          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 36       | 0.24          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 38       | 0.24          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 39       | 0.24          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 40       | 0.24          |
| (3,1781) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H   | 1        | 0.24          |
| (3,1781) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H   | 3        | 0.24          |
| (3,1781) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H   | 5        | 0.24          |
| (3,1781) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H   | 8        | 0.24          |
| (3,1781) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H   | 11       | 0.24          |
| (3,1781) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H   | 14       | 0.24          |
| (3,1781) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H   | 16       | 0.24          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA  | 11       | 0.24          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA  | 11       | 0.24          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA  | 11       | 0.24          |
| (3,1628) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2 | 30       | 0.24          |
| (3,1628) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2 | 30       | 0.24          |
| (3,1628) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2 | 30       | 0.24          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 2        | 0.24          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 4        | 0.24          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 11       | 0.24          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 24       | 0.24          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 38       | 0.24          |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 15       | 0.24          |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 15       | 0.24          |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 15       | 0.24          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H   | 14       | 0.24          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H   | 14       | 0.24          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H   | 14       | 0.24          |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 9        | 0.24          |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 9        | 0.24          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H    | 9        | 0.24          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 11       | 0.24          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 11       | 0.24          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 11       | 0.24          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 20       | 0.24          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 20       | 0.24          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 20       | 0.24          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 36       | 0.24          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 36       | 0.24          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 36       | 0.24          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 29       | 0.24          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 29       | 0.24          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 29       | 0.24          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 12       | 0.24          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 12       | 0.24          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 12       | 0.24          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 39       | 0.24          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 39       | 0.24          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 39       | 0.24          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 3        | 0.24          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 3        | 0.24          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 3        | 0.24          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 5        | 0.24          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 5        | 0.24          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 5        | 0.24          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 6        | 0.24          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 6        | 0.24          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 6        | 0.24          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 7        | 0.24          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 7        | 0.24          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 7        | 0.24          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 9        | 0.24          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 9        | 0.24          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 9        | 0.24          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 10       | 0.24          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 10       | 0.24          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 10       | 0.24          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 12       | 0.24          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 12       | 0.24          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 12       | 0.24          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 16       | 0.24          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 16       | 0.24          |

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| Key      | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|----------|--------------|-----------------|----------|---------------|
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 16       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 17       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 17       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 17       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 18       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 18       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 18       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 19       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 19       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 19       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 20       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 20       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 20       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 23       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 23       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 23       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 25       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 25       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 25       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 26       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 26       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 26       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 29       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 29       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 29       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 30       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 30       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 30       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 31       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 31       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 31       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 32       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 32       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 32       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 33       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 33       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 33       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 34       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 34       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 34       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 37       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 37       | 0.24          |

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| Key      | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|----------|--------------|-----------------|----------|---------------|
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 37       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 38       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 38       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 38       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 39       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 39       | 0.24          |
| (3,1204) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 39       | 0.24          |
| (3,1189) | 1:21:A:VAL:H | 1:100:A:GLU:HB3 | 3        | 0.24          |
| (3,1189) | 1:21:A:VAL:H | 1:100:A:GLU:HB3 | 28       | 0.24          |
| (3,1188) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 11       | 0.24          |
| (3,1188) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 15       | 0.24          |
| (3,1188) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 16       | 0.24          |
| (3,1188) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 18       | 0.24          |
| (3,1188) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 21       | 0.24          |
| (3,1188) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 24       | 0.24          |
| (3,1188) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 33       | 0.24          |
| (3,1188) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 35       | 0.24          |
| (3,1188) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 37       | 0.24          |
| (3,1188) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 39       | 0.24          |
| (3,1173) | 1:14:A:LYS:H | 1:14:A:LYS:HD2  | 11       | 0.24          |
| (3,1167) | 1:75:A:ASP:H | 1:74:A:ASP:HB2  | 37       | 0.24          |
| (3,919)  | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 5        | 0.24          |
| (3,919)  | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 30       | 0.24          |
| (3,889)  | 1:80:A:SER:H | 1:43:A:TYR:HB3  | 35       | 0.24          |
| (3,889)  | 1:80:A:SER:H | 1:43:A:TYR:HB3  | 37       | 0.24          |
| (3,870)  | 1:8:A:GLU:H  | 1:9:A:PRO:HD2   | 12       | 0.24          |
| (3,869)  | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 2        | 0.24          |
| (3,869)  | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 8        | 0.24          |
| (3,869)  | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 9        | 0.24          |
| (3,869)  | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 10       | 0.24          |
| (3,869)  | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 19       | 0.24          |
| (3,869)  | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 21       | 0.24          |
| (3,869)  | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 32       | 0.24          |
| (3,869)  | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 33       | 0.24          |
| (3,869)  | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 34       | 0.24          |
| (3,869)  | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 39       | 0.24          |
| (3,849)  | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 26       | 0.24          |
| (3,849)  | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 26       | 0.24          |
| (3,849)  | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 26       | 0.24          |
| (3,826)  | 1:17:A:GLN:H | 1:17:A:GLN:HG2  | 37       | 0.24          |
| (3,814)  | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 10       | 0.24          |
| (3,814)  | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 10       | 0.24          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 10       | 0.24          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 16       | 0.24          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 16       | 0.24          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 16       | 0.24          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 37       | 0.24          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 37       | 0.24          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 37       | 0.24          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 38       | 0.24          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 38       | 0.24          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 38       | 0.24          |
| (3,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 12       | 0.24          |
| (3,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 15       | 0.24          |
| (3,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 16       | 0.24          |
| (3,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 20       | 0.24          |
| (3,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 28       | 0.24          |
| (3,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 29       | 0.24          |
| (3,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 36       | 0.24          |
| (3,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2  | 11       | 0.24          |
| (3,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3  | 14       | 0.24          |
| (3,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3  | 17       | 0.24          |
| (3,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3  | 18       | 0.24          |
| (3,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3  | 20       | 0.24          |
| (3,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3  | 23       | 0.24          |
| (3,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3  | 26       | 0.24          |
| (3,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3  | 39       | 0.24          |
| (3,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3  | 40       | 0.24          |
| (3,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 1        | 0.24          |
| (3,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 2        | 0.24          |
| (3,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 4        | 0.24          |
| (3,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 18       | 0.24          |
| (3,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 21       | 0.24          |
| (3,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 22       | 0.24          |
| (3,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 25       | 0.24          |
| (3,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 27       | 0.24          |
| (3,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 29       | 0.24          |
| (3,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 30       | 0.24          |
| (3,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 33       | 0.24          |
| (3,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 35       | 0.24          |
| (3,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 38       | 0.24          |
| (3,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 39       | 0.24          |
| (3,590) | 1:3:A:ASP:H  | 1:2:A:ILE:HA    | 11       | 0.24          |
| (3,589) | 1:93:A:SER:H | 1:92:A:ARG:HG2  | 15       | 0.24          |

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| Key     | Atom-1       | Atom-2         | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1 | 35       | 0.24          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2 | 35       | 0.24          |
| (3,556) | 1:47:A:THR:H | 1:48:A:GLU:H   | 18       | 0.24          |
| (3,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA  | 28       | 0.24          |
| (3,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA  | 39       | 0.24          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H  | 5        | 0.24          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H  | 16       | 0.24          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H  | 29       | 0.24          |
| (3,513) | 1:67:A:THR:H | 1:66:A:MET:HG3 | 4        | 0.24          |
| (3,513) | 1:67:A:THR:H | 1:66:A:MET:HG3 | 15       | 0.24          |
| (3,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2 | 1        | 0.24          |
| (3,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2 | 7        | 0.24          |
| (3,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2 | 10       | 0.24          |
| (3,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2 | 26       | 0.24          |
| (3,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2 | 34       | 0.24          |
| (3,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2 | 39       | 0.24          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 3        | 0.24          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 4        | 0.24          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 6        | 0.24          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 9        | 0.24          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 10       | 0.24          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 11       | 0.24          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 12       | 0.24          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 13       | 0.24          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 14       | 0.24          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 16       | 0.24          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 17       | 0.24          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 18       | 0.24          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 19       | 0.24          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 21       | 0.24          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 23       | 0.24          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 24       | 0.24          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 25       | 0.24          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 26       | 0.24          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 27       | 0.24          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 29       | 0.24          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 30       | 0.24          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 31       | 0.24          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 32       | 0.24          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 34       | 0.24          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 35       | 0.24          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 36       | 0.24          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3  | 37       | 0.24          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3  | 38       | 0.24          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3  | 39       | 0.24          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3  | 40       | 0.24          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 34       | 0.24          |
| (3,365) | 1:18:A:ASN:H | 1:18:A:ASN:HB2  | 7        | 0.24          |
| (3,365) | 1:18:A:ASN:H | 1:18:A:ASN:HB2  | 22       | 0.24          |
| (3,365) | 1:18:A:ASN:H | 1:18:A:ASN:HB2  | 23       | 0.24          |
| (3,365) | 1:18:A:ASN:H | 1:18:A:ASN:HB2  | 31       | 0.24          |
| (3,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 32       | 0.24          |
| (3,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 34       | 0.24          |
| (3,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 38       | 0.24          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 2        | 0.24          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 2        | 0.24          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 15       | 0.24          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 15       | 0.24          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 32       | 0.24          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 32       | 0.24          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 33       | 0.24          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 33       | 0.24          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 35       | 0.24          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 35       | 0.24          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 38       | 0.24          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 38       | 0.24          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 39       | 0.24          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 39       | 0.24          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 1        | 0.24          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 3        | 0.24          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 5        | 0.24          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 7        | 0.24          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 8        | 0.24          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 11       | 0.24          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 14       | 0.24          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 17       | 0.24          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 19       | 0.24          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 21       | 0.24          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 24       | 0.24          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 25       | 0.24          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 27       | 0.24          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 28       | 0.24          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 30       | 0.24          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 32       | 0.24          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 33       | 0.24          |
| (3,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 35       | 0.24          |
| (3,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 37       | 0.24          |
| (3,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 40       | 0.24          |
| (3,135)  | 1:39:A:ILE:H   | 1:39:A:ILE:HG13 | 2        | 0.24          |
| (3,135)  | 1:39:A:ILE:H   | 1:39:A:ILE:HG13 | 24       | 0.24          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 4        | 0.24          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 4        | 0.24          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 4        | 0.24          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 14       | 0.24          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 14       | 0.24          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 14       | 0.24          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 22       | 0.24          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 22       | 0.24          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 22       | 0.24          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 32       | 0.24          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 32       | 0.24          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 32       | 0.24          |
| (3,22)   | 1:89:A:GLY:H   | 1:85:A:LEU:H    | 37       | 0.24          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 5        | 0.24          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 5        | 0.24          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 16       | 0.24          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 16       | 0.24          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 18       | 0.24          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 18       | 0.24          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 20       | 0.24          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 20       | 0.24          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 30       | 0.24          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 30       | 0.24          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 37       | 0.24          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 37       | 0.24          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 5        | 0.24          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 14       | 0.24          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 2        | 0.24          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 6        | 0.24          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 7        | 0.24          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 12       | 0.24          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 19       | 0.24          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 21       | 0.24          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 29       | 0.24          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 39       | 0.24          |
| (1,3159) | 1:42:A:TRP:HD1 | 1:42:A:TRP:HB3  | 40       | 0.24          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2 | 8        | 0.24          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2 | 8        | 0.24          |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2 | 9        | 0.24          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2 | 9        | 0.24          |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2 | 12       | 0.24          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2 | 12       | 0.24          |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2 | 24       | 0.24          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2 | 24       | 0.24          |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2 | 26       | 0.24          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2 | 26       | 0.24          |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2 | 27       | 0.24          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2 | 27       | 0.24          |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2 | 38       | 0.24          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2 | 38       | 0.24          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB2 | 27       | 0.24          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB3 | 27       | 0.24          |
| (1,3048) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2 | 7        | 0.24          |
| (1,3048) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2 | 18       | 0.24          |
| (1,3048) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2 | 25       | 0.24          |
| (1,3048) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2 | 34       | 0.24          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1 | 2        | 0.24          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1 | 6        | 0.24          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1 | 17       | 0.24          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 2        | 0.24          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 3        | 0.24          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 5        | 0.24          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 8        | 0.24          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 10       | 0.24          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 11       | 0.24          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 12       | 0.24          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 14       | 0.24          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 16       | 0.24          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 20       | 0.24          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 21       | 0.24          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 24       | 0.24          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 25       | 0.24          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 26       | 0.24          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 27       | 0.24          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 29       | 0.24          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 31       | 0.24          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 32       | 0.24          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 33       | 0.24          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 37       | 0.24          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H   | 40       | 0.24          |
| (1,2918) | 1:22:A:SER:HB2 | 1:25:A:GLN:H   | 8        | 0.24          |
| (1,2918) | 1:22:A:SER:HB2 | 1:25:A:GLN:H   | 17       | 0.24          |
| (1,2918) | 1:22:A:SER:HB2 | 1:25:A:GLN:H   | 22       | 0.24          |
| (1,2918) | 1:22:A:SER:HB2 | 1:25:A:GLN:H   | 23       | 0.24          |
| (1,2918) | 1:22:A:SER:HB2 | 1:25:A:GLN:H   | 24       | 0.24          |
| (1,2918) | 1:22:A:SER:HB2 | 1:25:A:GLN:H   | 26       | 0.24          |
| (1,2918) | 1:22:A:SER:HB2 | 1:25:A:GLN:H   | 30       | 0.24          |
| (1,2916) | 1:22:A:SER:HB2 | 1:22:A:SER:H   | 6        | 0.24          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3 | 8        | 0.24          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3 | 9        | 0.24          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3 | 12       | 0.24          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3 | 15       | 0.24          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3 | 20       | 0.24          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3 | 28       | 0.24          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3 | 29       | 0.24          |
| (1,2742) | 1:86:A:GLU:HG2 | 1:86:A:GLU:HG3 | 35       | 0.24          |
| (1,2718) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 13       | 0.24          |
| (1,2718) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 14       | 0.24          |
| (1,2718) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 15       | 0.24          |
| (1,2718) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 22       | 0.24          |
| (1,2718) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 26       | 0.24          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 6        | 0.24          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 8        | 0.24          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 12       | 0.24          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 13       | 0.24          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 19       | 0.24          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 28       | 0.24          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 29       | 0.24          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 33       | 0.24          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 35       | 0.24          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 36       | 0.24          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 40       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 1        | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 2        | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 3        | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 4        | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 5        | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 6        | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 7        | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 8        | 0.24          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 9        | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 10       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 11       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 12       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 13       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 14       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 15       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 16       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 17       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 18       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 19       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 20       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 21       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 22       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 23       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 24       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 25       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 26       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 27       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 28       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 29       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 30       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 31       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 32       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 33       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 34       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 35       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 36       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 37       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 38       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 39       | 0.24          |
| (1,2667) | 1:25:A:GLN:HG2 | 1:25:A:GLN:HG3 | 40       | 0.24          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3  | 1        | 0.24          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3  | 4        | 0.24          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3  | 6        | 0.24          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3  | 7        | 0.24          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3  | 14       | 0.24          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3  | 17       | 0.24          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3  | 20       | 0.24          |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 5        | 0.24          |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 30       | 0.24          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 21       | 0.24          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2539) | 1:73:A:PRO:HG2  | 1:73:A:PRO:HA  | 22       | 0.24          |
| (1,2539) | 1:73:A:PRO:HG2  | 1:73:A:PRO:HA  | 24       | 0.24          |
| (1,2539) | 1:73:A:PRO:HG2  | 1:73:A:PRO:HA  | 25       | 0.24          |
| (1,2539) | 1:73:A:PRO:HG2  | 1:73:A:PRO:HA  | 29       | 0.24          |
| (1,2539) | 1:73:A:PRO:HG2  | 1:73:A:PRO:HA  | 32       | 0.24          |
| (1,2539) | 1:73:A:PRO:HG2  | 1:73:A:PRO:HA  | 33       | 0.24          |
| (1,2539) | 1:73:A:PRO:HG2  | 1:73:A:PRO:HA  | 34       | 0.24          |
| (1,2539) | 1:73:A:PRO:HG2  | 1:73:A:PRO:HA  | 35       | 0.24          |
| (1,2539) | 1:73:A:PRO:HG2  | 1:73:A:PRO:HA  | 38       | 0.24          |
| (1,2539) | 1:73:A:PRO:HG2  | 1:73:A:PRO:HA  | 39       | 0.24          |
| (1,2534) | 1:73:A:PRO:HD3  | 1:73:A:PRO:HB3 | 18       | 0.24          |
| (1,2512) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD3 | 11       | 0.24          |
| (1,2485) | 1:9:A:PRO:HD2   | 1:9:A:PRO:HB3  | 28       | 0.24          |
| (1,2479) | 1:9:A:PRO:HD2   | 1:8:A:GLU:HA   | 16       | 0.24          |
| (1,2467) | 1:4:A:PRO:HB2   | 1:4:A:PRO:HD2  | 15       | 0.24          |
| (1,2431) | 1:82:A:ILE:HB   | 1:41:A:THR:H   | 17       | 0.24          |
| (1,2431) | 1:82:A:ILE:HB   | 1:41:A:THR:H   | 34       | 0.24          |
| (1,2322) | 1:80:A:SER:HB2  | 1:81:A:VAL:H   | 6        | 0.24          |
| (1,2322) | 1:80:A:SER:HB2  | 1:81:A:VAL:H   | 14       | 0.24          |
| (1,2322) | 1:80:A:SER:HB2  | 1:81:A:VAL:H   | 39       | 0.24          |
| (1,2285) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H   | 3        | 0.24          |
| (1,2285) | 1:96:A:GLU:HG3  | 1:97:A:LEU:H   | 5        | 0.24          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1 | 1        | 0.24          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2 | 1        | 0.24          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1 | 19       | 0.24          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2 | 19       | 0.24          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1 | 28       | 0.24          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2 | 28       | 0.24          |
| (1,2213) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 2        | 0.24          |
| (1,2213) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 6        | 0.24          |
| (1,2213) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 7        | 0.24          |
| (1,2213) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 12       | 0.24          |
| (1,2213) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 19       | 0.24          |
| (1,2213) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 21       | 0.24          |
| (1,2213) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 29       | 0.24          |
| (1,2213) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 39       | 0.24          |
| (1,2213) | 1:42:A:TRP:HB3  | 1:42:A:TRP:HD1 | 40       | 0.24          |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H   | 20       | 0.24          |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H   | 21       | 0.24          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 3        | 0.24          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 3        | 0.24          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 3        | 0.24          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 4        | 0.24          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 4        | 0.24          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 4        | 0.24          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 6        | 0.24          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 6        | 0.24          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 6        | 0.24          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 7        | 0.24          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 7        | 0.24          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 7        | 0.24          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 10       | 0.24          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 10       | 0.24          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 10       | 0.24          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 11       | 0.24          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 11       | 0.24          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 11       | 0.24          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 16       | 0.24          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 16       | 0.24          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 16       | 0.24          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 32       | 0.24          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 32       | 0.24          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 32       | 0.24          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 34       | 0.24          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 34       | 0.24          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 34       | 0.24          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 36       | 0.24          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 36       | 0.24          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 36       | 0.24          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 38       | 0.24          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 38       | 0.24          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 38       | 0.24          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 2        | 0.24          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 2        | 0.24          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 2        | 0.24          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 5        | 0.24          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 5        | 0.24          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 5        | 0.24          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 5        | 0.24          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 5        | 0.24          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 5        | 0.24          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 23       | 0.24          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 23       | 0.24          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 23       | 0.24          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 23       | 0.24          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 23       | 0.24          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 23       | 0.24          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 25       | 0.24          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 25       | 0.24          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 25       | 0.24          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 25       | 0.24          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 25       | 0.24          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 25       | 0.24          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 5        | 0.24          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 5        | 0.24          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 5        | 0.24          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 7        | 0.24          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 7        | 0.24          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 7        | 0.24          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 26       | 0.24          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 26       | 0.24          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 26       | 0.24          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 32       | 0.24          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 32       | 0.24          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 32       | 0.24          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 3        | 0.24          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 4        | 0.24          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 5        | 0.24          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 7        | 0.24          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 10       | 0.24          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 13       | 0.24          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 14       | 0.24          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 15       | 0.24          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 17       | 0.24          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 19       | 0.24          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 20       | 0.24          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 21       | 0.24          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 22       | 0.24          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 23       | 0.24          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 24       | 0.24          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 25       | 0.24          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 29       | 0.24          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 30       | 0.24          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 31       | 0.24          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 32       | 0.24          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 34       | 0.24          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 35       | 0.24          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 36       | 0.24          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 38       | 0.24          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 39       | 0.24          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 40       | 0.24          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 15       | 0.24          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 18       | 0.24          |
| (1,1959) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 27       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 2        | 0.24          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 2        | 0.24          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 2        | 0.24          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 3        | 0.24          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 3        | 0.24          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 3        | 0.24          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 4        | 0.24          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 4        | 0.24          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 4        | 0.24          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 7        | 0.24          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 7        | 0.24          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 7        | 0.24          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 10       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 10       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 10       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 11       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 11       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 11       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 12       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 12       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 12       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 16       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 16       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 16       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 18       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 18       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 18       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 19       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 19       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 19       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 21       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 21       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 21       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 22       | 0.24          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA   | 22       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA   | 22       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA   | 24       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA   | 24       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA   | 24       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA   | 26       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA   | 26       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA   | 26       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA   | 28       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA   | 28       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA   | 28       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA   | 29       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA   | 29       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA   | 29       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA   | 31       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA   | 31       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA   | 31       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA   | 32       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA   | 32       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA   | 32       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA   | 36       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA   | 36       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA   | 36       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA   | 37       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA   | 37       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA   | 37       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA   | 38       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA   | 38       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA   | 38       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA   | 39       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA   | 39       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA   | 39       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA   | 40       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA   | 40       | 0.24          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA   | 40       | 0.24          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2  | 1        | 0.24          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2  | 7        | 0.24          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2  | 16       | 0.24          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 3        | 0.24          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 3        | 0.24          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 3        | 0.24          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 3        | 0.24          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 3        | 0.24          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 3        | 0.24          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 3        | 0.24          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 3        | 0.24          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 3        | 0.24          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 8        | 0.24          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 8        | 0.24          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 8        | 0.24          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 8        | 0.24          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 8        | 0.24          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 8        | 0.24          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 8        | 0.24          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 8        | 0.24          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 8        | 0.24          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 14       | 0.24          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 14       | 0.24          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 14       | 0.24          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 14       | 0.24          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 14       | 0.24          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 14       | 0.24          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 14       | 0.24          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 14       | 0.24          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 14       | 0.24          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 26       | 0.24          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 26       | 0.24          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 26       | 0.24          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 26       | 0.24          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 26       | 0.24          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 26       | 0.24          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 26       | 0.24          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 26       | 0.24          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 26       | 0.24          |
| (1,1904) | 1:66:A:MET:HE1  | 1:43:A:TYR:H    | 12       | 0.24          |
| (1,1904) | 1:66:A:MET:HE2  | 1:43:A:TYR:H    | 12       | 0.24          |
| (1,1904) | 1:66:A:MET:HE3  | 1:43:A:TYR:H    | 12       | 0.24          |
| (1,1904) | 1:66:A:MET:HE1  | 1:43:A:TYR:H    | 19       | 0.24          |
| (1,1904) | 1:66:A:MET:HE2  | 1:43:A:TYR:H    | 19       | 0.24          |
| (1,1904) | 1:66:A:MET:HE3  | 1:43:A:TYR:H    | 19       | 0.24          |
| (1,1904) | 1:66:A:MET:HE1  | 1:43:A:TYR:H    | 39       | 0.24          |
| (1,1904) | 1:66:A:MET:HE2  | 1:43:A:TYR:H    | 39       | 0.24          |
| (1,1904) | 1:66:A:MET:HE3  | 1:43:A:TYR:H    | 39       | 0.24          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2  | 3        | 0.24          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 4        | 0.24          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 5        | 0.24          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 7        | 0.24          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 10       | 0.24          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 13       | 0.24          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 14       | 0.24          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 15       | 0.24          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 17       | 0.24          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 19       | 0.24          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 20       | 0.24          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 21       | 0.24          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 22       | 0.24          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 23       | 0.24          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 24       | 0.24          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 25       | 0.24          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 29       | 0.24          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 30       | 0.24          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 31       | 0.24          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 32       | 0.24          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 34       | 0.24          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 35       | 0.24          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 36       | 0.24          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 38       | 0.24          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 39       | 0.24          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 40       | 0.24          |
| (1,1778) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H   | 1        | 0.24          |
| (1,1778) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H   | 3        | 0.24          |
| (1,1778) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H   | 5        | 0.24          |
| (1,1778) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H   | 8        | 0.24          |
| (1,1778) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H   | 11       | 0.24          |
| (1,1778) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H   | 14       | 0.24          |
| (1,1778) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H   | 16       | 0.24          |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA  | 11       | 0.24          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA  | 11       | 0.24          |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA  | 11       | 0.24          |
| (1,1624) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2 | 30       | 0.24          |
| (1,1624) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2 | 30       | 0.24          |
| (1,1624) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2 | 30       | 0.24          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 2        | 0.24          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 4        | 0.24          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 11       | 0.24          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 24       | 0.24          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 38       | 0.24          |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3  | 15       | 0.24          |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3  | 15       | 0.24          |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3  | 15       | 0.24          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H    | 14       | 0.24          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H    | 14       | 0.24          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H    | 14       | 0.24          |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H    | 9        | 0.24          |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H    | 9        | 0.24          |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H    | 9        | 0.24          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 11       | 0.24          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 11       | 0.24          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 11       | 0.24          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 20       | 0.24          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 20       | 0.24          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 20       | 0.24          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 36       | 0.24          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 36       | 0.24          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 36       | 0.24          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 29       | 0.24          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 29       | 0.24          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 29       | 0.24          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 12       | 0.24          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 12       | 0.24          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 12       | 0.24          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 39       | 0.24          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 39       | 0.24          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 39       | 0.24          |
| (1,1237) | 1:13:A:THR:HG21 | 1:34:A:SER:HB2  | 26       | 0.24          |
| (1,1237) | 1:13:A:THR:HG22 | 1:34:A:SER:HB2  | 26       | 0.24          |
| (1,1237) | 1:13:A:THR:HG23 | 1:34:A:SER:HB2  | 26       | 0.24          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 3        | 0.24          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 3        | 0.24          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 3        | 0.24          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 5        | 0.24          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 5        | 0.24          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 5        | 0.24          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 6        | 0.24          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 6        | 0.24          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 6        | 0.24          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 7        | 0.24          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 7        | 0.24          |

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| Key      | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|----------|--------------|-----------------|----------|---------------|
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 7        | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 9        | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 9        | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 9        | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 10       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 10       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 10       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 12       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 12       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 12       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 16       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 16       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 16       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 17       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 17       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 17       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 18       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 18       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 18       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 19       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 19       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 19       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 20       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 20       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 20       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 23       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 23       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 23       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 25       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 25       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 25       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 26       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 26       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 26       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 29       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 29       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 29       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 30       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 30       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 30       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 31       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 31       | 0.24          |

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| Key      | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|----------|--------------|-----------------|----------|---------------|
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 31       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 32       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 32       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 32       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 33       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 33       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 33       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 34       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 34       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 34       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 37       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 37       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 37       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 38       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 38       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 38       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG21 | 39       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG22 | 39       | 0.24          |
| (1,1200) | 1:39:A:ILE:H | 1:39:A:ILE:HG23 | 39       | 0.24          |
| (1,1185) | 1:21:A:VAL:H | 1:100:A:GLU:HB3 | 3        | 0.24          |
| (1,1185) | 1:21:A:VAL:H | 1:100:A:GLU:HB3 | 28       | 0.24          |
| (1,1184) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 11       | 0.24          |
| (1,1184) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 15       | 0.24          |
| (1,1184) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 16       | 0.24          |
| (1,1184) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 18       | 0.24          |
| (1,1184) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 21       | 0.24          |
| (1,1184) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 24       | 0.24          |
| (1,1184) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 33       | 0.24          |
| (1,1184) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 35       | 0.24          |
| (1,1184) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 37       | 0.24          |
| (1,1184) | 1:19:A:ILE:H | 1:97:A:LEU:HA   | 39       | 0.24          |
| (1,1169) | 1:14:A:LYS:H | 1:14:A:LYS:HD2  | 11       | 0.24          |
| (1,1163) | 1:75:A:ASP:H | 1:74:A:ASP:HB2  | 37       | 0.24          |
| (1,918)  | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 5        | 0.24          |
| (1,918)  | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 30       | 0.24          |
| (1,888)  | 1:80:A:SER:H | 1:43:A:TYR:HB3  | 35       | 0.24          |
| (1,888)  | 1:80:A:SER:H | 1:43:A:TYR:HB3  | 37       | 0.24          |
| (1,870)  | 1:8:A:GLU:H  | 1:9:A:PRO:HD2   | 12       | 0.24          |
| (1,869)  | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 2        | 0.24          |
| (1,869)  | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 8        | 0.24          |
| (1,869)  | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 9        | 0.24          |
| (1,869)  | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 10       | 0.24          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 19       | 0.24          |
| (1,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 21       | 0.24          |
| (1,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 32       | 0.24          |
| (1,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 33       | 0.24          |
| (1,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 34       | 0.24          |
| (1,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 39       | 0.24          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 26       | 0.24          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 26       | 0.24          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 26       | 0.24          |
| (1,826) | 1:17:A:GLN:H | 1:17:A:GLN:HG2  | 37       | 0.24          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 10       | 0.24          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 10       | 0.24          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 10       | 0.24          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 16       | 0.24          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 16       | 0.24          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 16       | 0.24          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 37       | 0.24          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 37       | 0.24          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 37       | 0.24          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 38       | 0.24          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 38       | 0.24          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 38       | 0.24          |
| (1,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 12       | 0.24          |
| (1,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 15       | 0.24          |
| (1,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 16       | 0.24          |
| (1,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 20       | 0.24          |
| (1,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 28       | 0.24          |
| (1,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 29       | 0.24          |
| (1,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 36       | 0.24          |
| (1,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2  | 11       | 0.24          |
| (1,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3  | 14       | 0.24          |
| (1,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3  | 17       | 0.24          |
| (1,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3  | 18       | 0.24          |
| (1,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3  | 20       | 0.24          |
| (1,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3  | 23       | 0.24          |
| (1,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3  | 26       | 0.24          |
| (1,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3  | 39       | 0.24          |
| (1,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3  | 40       | 0.24          |
| (1,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 1        | 0.24          |
| (1,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 2        | 0.24          |
| (1,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 4        | 0.24          |
| (1,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3  | 18       | 0.24          |

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| Key     | Atom-1       | Atom-2         | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (1,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3 | 21       | 0.24          |
| (1,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3 | 22       | 0.24          |
| (1,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3 | 25       | 0.24          |
| (1,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3 | 27       | 0.24          |
| (1,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3 | 29       | 0.24          |
| (1,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3 | 30       | 0.24          |
| (1,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3 | 33       | 0.24          |
| (1,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3 | 35       | 0.24          |
| (1,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3 | 38       | 0.24          |
| (1,685) | 1:23:A:GLU:H | 1:23:A:GLU:HG3 | 39       | 0.24          |
| (1,590) | 1:3:A:ASP:H  | 1:2:A:ILE:HA   | 11       | 0.24          |
| (1,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1 | 35       | 0.24          |
| (1,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2 | 35       | 0.24          |
| (1,556) | 1:47:A:THR:H | 1:48:A:GLU:H   | 18       | 0.24          |
| (1,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA  | 28       | 0.24          |
| (1,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA  | 39       | 0.24          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H  | 5        | 0.24          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H  | 16       | 0.24          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H  | 29       | 0.24          |
| (1,513) | 1:67:A:THR:H | 1:66:A:MET:HG3 | 4        | 0.24          |
| (1,513) | 1:67:A:THR:H | 1:66:A:MET:HG3 | 15       | 0.24          |
| (1,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2 | 1        | 0.24          |
| (1,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2 | 7        | 0.24          |
| (1,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2 | 10       | 0.24          |
| (1,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2 | 26       | 0.24          |
| (1,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2 | 34       | 0.24          |
| (1,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2 | 39       | 0.24          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 3        | 0.24          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 4        | 0.24          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 6        | 0.24          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 9        | 0.24          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 10       | 0.24          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 11       | 0.24          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 12       | 0.24          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 13       | 0.24          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 14       | 0.24          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 16       | 0.24          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 17       | 0.24          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 18       | 0.24          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 19       | 0.24          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 21       | 0.24          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3 | 23       | 0.24          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3  | 24       | 0.24          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3  | 25       | 0.24          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3  | 26       | 0.24          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3  | 27       | 0.24          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3  | 29       | 0.24          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3  | 30       | 0.24          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3  | 31       | 0.24          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3  | 32       | 0.24          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3  | 34       | 0.24          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3  | 35       | 0.24          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3  | 36       | 0.24          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3  | 37       | 0.24          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3  | 38       | 0.24          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3  | 39       | 0.24          |
| (1,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3  | 40       | 0.24          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 34       | 0.24          |
| (1,365) | 1:18:A:ASN:H | 1:18:A:ASN:HB2  | 7        | 0.24          |
| (1,365) | 1:18:A:ASN:H | 1:18:A:ASN:HB2  | 22       | 0.24          |
| (1,365) | 1:18:A:ASN:H | 1:18:A:ASN:HB2  | 23       | 0.24          |
| (1,365) | 1:18:A:ASN:H | 1:18:A:ASN:HB2  | 31       | 0.24          |
| (1,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 32       | 0.24          |
| (1,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 34       | 0.24          |
| (1,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 38       | 0.24          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 2        | 0.24          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 2        | 0.24          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 15       | 0.24          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 15       | 0.24          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 32       | 0.24          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 32       | 0.24          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 33       | 0.24          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 33       | 0.24          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 35       | 0.24          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 35       | 0.24          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 38       | 0.24          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 38       | 0.24          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 39       | 0.24          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 39       | 0.24          |
| (1,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 1        | 0.24          |
| (1,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 3        | 0.24          |
| (1,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 5        | 0.24          |
| (1,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 7        | 0.24          |
| (1,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 8        | 0.24          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 11       | 0.24          |
| (1,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 14       | 0.24          |
| (1,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 17       | 0.24          |
| (1,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 19       | 0.24          |
| (1,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 21       | 0.24          |
| (1,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 24       | 0.24          |
| (1,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 25       | 0.24          |
| (1,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 27       | 0.24          |
| (1,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 28       | 0.24          |
| (1,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 30       | 0.24          |
| (1,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 32       | 0.24          |
| (1,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 33       | 0.24          |
| (1,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 35       | 0.24          |
| (1,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 37       | 0.24          |
| (1,169)  | 1:10:A:ILE:H   | 1:10:A:ILE:HG12 | 40       | 0.24          |
| (1,149)  | 1:45:A:GLY:H   | 1:46:A:PRO:HD3  | 12       | 0.24          |
| (1,133)  | 1:39:A:ILE:H   | 1:39:A:ILE:HG13 | 2        | 0.24          |
| (1,133)  | 1:39:A:ILE:H   | 1:39:A:ILE:HG13 | 24       | 0.24          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 4        | 0.24          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 4        | 0.24          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 4        | 0.24          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 14       | 0.24          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 14       | 0.24          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 14       | 0.24          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 22       | 0.24          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 22       | 0.24          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 22       | 0.24          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 32       | 0.24          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 32       | 0.24          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 32       | 0.24          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 17       | 0.23          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 17       | 0.23          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 28       | 0.23          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 28       | 0.23          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 31       | 0.23          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 31       | 0.23          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 2        | 0.23          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 2        | 0.23          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 2        | 0.23          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 2        | 0.23          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 2        | 0.23          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 2        | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,3133) | 1:55:A:TYR:HD1  | 1:49:A:LEU:HB2  | 2        | 0.23          |
| (3,3133) | 1:55:A:TYR:HD2  | 1:49:A:LEU:HB2  | 2        | 0.23          |
| (3,3133) | 1:55:A:TYR:HD1  | 1:49:A:LEU:HB2  | 5        | 0.23          |
| (3,3133) | 1:55:A:TYR:HD2  | 1:49:A:LEU:HB2  | 5        | 0.23          |
| (3,3133) | 1:55:A:TYR:HD1  | 1:49:A:LEU:HB2  | 11       | 0.23          |
| (3,3133) | 1:55:A:TYR:HD2  | 1:49:A:LEU:HB2  | 11       | 0.23          |
| (3,3133) | 1:55:A:TYR:HD1  | 1:49:A:LEU:HB2  | 13       | 0.23          |
| (3,3133) | 1:55:A:TYR:HD2  | 1:49:A:LEU:HB2  | 13       | 0.23          |
| (3,3133) | 1:55:A:TYR:HD1  | 1:49:A:LEU:HB2  | 18       | 0.23          |
| (3,3133) | 1:55:A:TYR:HD2  | 1:49:A:LEU:HB2  | 18       | 0.23          |
| (3,3133) | 1:55:A:TYR:HD1  | 1:49:A:LEU:HB2  | 21       | 0.23          |
| (3,3133) | 1:55:A:TYR:HD2  | 1:49:A:LEU:HB2  | 21       | 0.23          |
| (3,3133) | 1:55:A:TYR:HD1  | 1:49:A:LEU:HB2  | 30       | 0.23          |
| (3,3133) | 1:55:A:TYR:HD2  | 1:49:A:LEU:HB2  | 30       | 0.23          |
| (3,3090) | 1:98:A:LYS:HD3  | 1:20:A:VAL:HG21 | 5        | 0.23          |
| (3,3090) | 1:98:A:LYS:HD3  | 1:20:A:VAL:HG22 | 5        | 0.23          |
| (3,3090) | 1:98:A:LYS:HD3  | 1:20:A:VAL:HG23 | 5        | 0.23          |
| (3,3056) | 1:60:A:ASP:HB2  | 1:63:A:CYS:HB2  | 11       | 0.23          |
| (3,3056) | 1:60:A:ASP:HB2  | 1:63:A:CYS:HB2  | 27       | 0.23          |
| (3,3055) | 1:57:A:PHE:HB3  | 1:42:A:TRP:HE1  | 29       | 0.23          |
| (3,3054) | 1:57:A:PHE:HB3  | 1:57:A:PHE:H    | 4        | 0.23          |
| (3,3054) | 1:57:A:PHE:HB3  | 1:57:A:PHE:H    | 6        | 0.23          |
| (3,3054) | 1:57:A:PHE:HB3  | 1:57:A:PHE:H    | 7        | 0.23          |
| (3,3054) | 1:57:A:PHE:HB3  | 1:57:A:PHE:H    | 17       | 0.23          |
| (3,3054) | 1:57:A:PHE:HB3  | 1:57:A:PHE:H    | 19       | 0.23          |
| (3,3054) | 1:57:A:PHE:HB3  | 1:57:A:PHE:H    | 28       | 0.23          |
| (3,3054) | 1:57:A:PHE:HB3  | 1:57:A:PHE:H    | 34       | 0.23          |
| (3,3054) | 1:57:A:PHE:HB3  | 1:57:A:PHE:H    | 35       | 0.23          |
| (3,3054) | 1:57:A:PHE:HB3  | 1:57:A:PHE:H    | 36       | 0.23          |
| (3,3054) | 1:57:A:PHE:HB3  | 1:57:A:PHE:H    | 39       | 0.23          |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG21 | 20       | 0.23          |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG22 | 20       | 0.23          |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG23 | 20       | 0.23          |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG21 | 27       | 0.23          |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG22 | 27       | 0.23          |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG23 | 27       | 0.23          |
| (3,2938) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 5        | 0.23          |
| (3,2925) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 5        | 0.23          |
| (3,2925) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 27       | 0.23          |
| (3,2925) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 39       | 0.23          |
| (3,2923) | 1:22:A:SER:HB2  | 1:22:A:SER:H    | 7        | 0.23          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 1        | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 2        | 0.23          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 3        | 0.23          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 4        | 0.23          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 5        | 0.23          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 6        | 0.23          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 7        | 0.23          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 8        | 0.23          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 9        | 0.23          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 10       | 0.23          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 11       | 0.23          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 14       | 0.23          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 15       | 0.23          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 16       | 0.23          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 18       | 0.23          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 21       | 0.23          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 23       | 0.23          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 25       | 0.23          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 26       | 0.23          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 27       | 0.23          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 29       | 0.23          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 31       | 0.23          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 32       | 0.23          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 33       | 0.23          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 35       | 0.23          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 36       | 0.23          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 37       | 0.23          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 38       | 0.23          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 39       | 0.23          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 40       | 0.23          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 1        | 0.23          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 2        | 0.23          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 3        | 0.23          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 4        | 0.23          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 5        | 0.23          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 6        | 0.23          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 7        | 0.23          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 8        | 0.23          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 9        | 0.23          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 10       | 0.23          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 11       | 0.23          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 14       | 0.23          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 15       | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 16       | 0.23          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 18       | 0.23          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 21       | 0.23          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 23       | 0.23          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 25       | 0.23          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 26       | 0.23          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 27       | 0.23          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 29       | 0.23          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 31       | 0.23          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 32       | 0.23          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 33       | 0.23          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 35       | 0.23          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 36       | 0.23          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 37       | 0.23          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 38       | 0.23          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 39       | 0.23          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 40       | 0.23          |
| (3,2748) | 1:86:A:GLU:HG3  | 1:87:A:PRO:HA   | 12       | 0.23          |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 2        | 0.23          |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 3        | 0.23          |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 5        | 0.23          |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 6        | 0.23          |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 8        | 0.23          |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 9        | 0.23          |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 10       | 0.23          |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 11       | 0.23          |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 12       | 0.23          |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 18       | 0.23          |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 21       | 0.23          |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 24       | 0.23          |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 25       | 0.23          |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 27       | 0.23          |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 29       | 0.23          |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 30       | 0.23          |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 31       | 0.23          |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 34       | 0.23          |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 35       | 0.23          |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 36       | 0.23          |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 37       | 0.23          |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 38       | 0.23          |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 39       | 0.23          |
| (3,2697) | 1:23:A:GLU:HA   | 1:24:A:HIS:H    | 1        | 0.23          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 2        | 0.23          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 3        | 0.23          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 4        | 0.23          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 5        | 0.23          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 9        | 0.23          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 11       | 0.23          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 14       | 0.23          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 15       | 0.23          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 16       | 0.23          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 17       | 0.23          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 20       | 0.23          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 21       | 0.23          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 22       | 0.23          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 24       | 0.23          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 25       | 0.23          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 26       | 0.23          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 27       | 0.23          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 30       | 0.23          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 32       | 0.23          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 34       | 0.23          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 38       | 0.23          |
| (3,2676) | 1:25:A:GLN:HG3 | 1:22:A:SER:HB2 | 7        | 0.23          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 5        | 0.23          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 9        | 0.23          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 10       | 0.23          |
| (3,2653) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H   | 28       | 0.23          |
| (3,2653) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H   | 29       | 0.23          |
| (3,2602) | 1:36:A:ASP:HB2 | 1:37:A:ASP:H   | 40       | 0.23          |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 2        | 0.23          |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 6        | 0.23          |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 10       | 0.23          |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 19       | 0.23          |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 20       | 0.23          |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 28       | 0.23          |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 32       | 0.23          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 23       | 0.23          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 36       | 0.23          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 37       | 0.23          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 40       | 0.23          |
| (3,2538) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 7        | 0.23          |
| (3,2538) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 8        | 0.23          |
| (3,2538) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 12       | 0.23          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,2538) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3  | 13       | 0.23          |
| (3,2485) | 1:9:A:PRO:HD3  | 1:9:A:PRO:HB3   | 21       | 0.23          |
| (3,2485) | 1:9:A:PRO:HD3  | 1:9:A:PRO:HB3   | 24       | 0.23          |
| (3,2485) | 1:9:A:PRO:HD3  | 1:9:A:PRO:HB3   | 25       | 0.23          |
| (3,2485) | 1:9:A:PRO:HD3  | 1:9:A:PRO:HB3   | 36       | 0.23          |
| (3,2485) | 1:9:A:PRO:HD3  | 1:9:A:PRO:HB3   | 39       | 0.23          |
| (3,2470) | 1:4:A:PRO:HB2  | 1:4:A:PRO:HD2   | 17       | 0.23          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ   | 34       | 0.23          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ   | 34       | 0.23          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ   | 34       | 0.23          |
| (3,2327) | 1:80:A:SER:HB2 | 1:94:A:THR:HG21 | 28       | 0.23          |
| (3,2327) | 1:80:A:SER:HB2 | 1:94:A:THR:HG22 | 28       | 0.23          |
| (3,2327) | 1:80:A:SER:HB2 | 1:94:A:THR:HG23 | 28       | 0.23          |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H    | 1        | 0.23          |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H    | 18       | 0.23          |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H    | 20       | 0.23          |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H    | 23       | 0.23          |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H    | 25       | 0.23          |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H    | 30       | 0.23          |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H    | 32       | 0.23          |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H    | 36       | 0.23          |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H    | 6        | 0.23          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 25       | 0.23          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 25       | 0.23          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 34       | 0.23          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 34       | 0.23          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 38       | 0.23          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 38       | 0.23          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 40       | 0.23          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 40       | 0.23          |
| (3,2173) | 1:43:A:TYR:HA  | 1:80:A:SER:H    | 2        | 0.23          |
| (3,2173) | 1:43:A:TYR:HA  | 1:80:A:SER:H    | 4        | 0.23          |
| (3,2173) | 1:43:A:TYR:HA  | 1:80:A:SER:H    | 16       | 0.23          |
| (3,2173) | 1:43:A:TYR:HA  | 1:80:A:SER:H    | 18       | 0.23          |
| (3,2173) | 1:43:A:TYR:HA  | 1:80:A:SER:H    | 19       | 0.23          |
| (3,2173) | 1:43:A:TYR:HA  | 1:80:A:SER:H    | 37       | 0.23          |
| (3,2173) | 1:43:A:TYR:HA  | 1:80:A:SER:H    | 39       | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3   | 1        | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3   | 2        | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3   | 3        | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3   | 4        | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3   | 5        | 0.23          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 6        | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 7        | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 8        | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 9        | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 10       | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 11       | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 12       | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 13       | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 14       | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 15       | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 17       | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 18       | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 19       | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 20       | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 21       | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 22       | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 23       | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 24       | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 25       | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 26       | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 27       | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 28       | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 29       | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 30       | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 31       | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 32       | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 34       | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 35       | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 36       | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 37       | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 38       | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 39       | 0.23          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 40       | 0.23          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 8        | 0.23          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 8        | 0.23          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 8        | 0.23          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 9        | 0.23          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 9        | 0.23          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 9        | 0.23          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 16       | 0.23          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 16       | 0.23          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 16       | 0.23          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 18       | 0.23          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 18       | 0.23          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 18       | 0.23          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 20       | 0.23          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 20       | 0.23          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 20       | 0.23          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 27       | 0.23          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 27       | 0.23          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 27       | 0.23          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 28       | 0.23          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 28       | 0.23          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 28       | 0.23          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 31       | 0.23          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 31       | 0.23          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 31       | 0.23          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 32       | 0.23          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 32       | 0.23          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 32       | 0.23          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 38       | 0.23          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 38       | 0.23          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 38       | 0.23          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 40       | 0.23          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 40       | 0.23          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 40       | 0.23          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA | 9        | 0.23          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA | 9        | 0.23          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA | 9        | 0.23          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA | 14       | 0.23          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA | 14       | 0.23          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA | 14       | 0.23          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA | 19       | 0.23          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA | 19       | 0.23          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA | 19       | 0.23          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA | 23       | 0.23          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA | 23       | 0.23          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA | 23       | 0.23          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA | 25       | 0.23          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA | 25       | 0.23          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA | 25       | 0.23          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA | 26       | 0.23          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA | 26       | 0.23          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA | 26       | 0.23          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 27       | 0.23          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 27       | 0.23          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 27       | 0.23          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 29       | 0.23          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 29       | 0.23          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 29       | 0.23          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 30       | 0.23          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 30       | 0.23          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 30       | 0.23          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 33       | 0.23          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 33       | 0.23          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 33       | 0.23          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 17       | 0.23          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 17       | 0.23          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 17       | 0.23          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 17       | 0.23          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 17       | 0.23          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 17       | 0.23          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 18       | 0.23          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 18       | 0.23          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 18       | 0.23          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 18       | 0.23          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 18       | 0.23          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 18       | 0.23          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 22       | 0.23          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 22       | 0.23          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 22       | 0.23          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 22       | 0.23          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 22       | 0.23          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 22       | 0.23          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 27       | 0.23          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 27       | 0.23          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 27       | 0.23          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 27       | 0.23          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 27       | 0.23          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 27       | 0.23          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 32       | 0.23          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 32       | 0.23          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 32       | 0.23          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 32       | 0.23          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 32       | 0.23          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 32       | 0.23          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 36       | 0.23          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 36       | 0.23          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 36       | 0.23          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 36       | 0.23          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 36       | 0.23          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 36       | 0.23          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 14       | 0.23          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 14       | 0.23          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 14       | 0.23          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 29       | 0.23          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 29       | 0.23          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 29       | 0.23          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 40       | 0.23          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 40       | 0.23          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 40       | 0.23          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 13       | 0.23          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 13       | 0.23          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 13       | 0.23          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 18       | 0.23          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 18       | 0.23          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 18       | 0.23          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 25       | 0.23          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 25       | 0.23          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 25       | 0.23          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 27       | 0.23          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 27       | 0.23          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 27       | 0.23          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 30       | 0.23          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 30       | 0.23          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 30       | 0.23          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 34       | 0.23          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 34       | 0.23          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 34       | 0.23          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 36       | 0.23          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 36       | 0.23          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 36       | 0.23          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 37       | 0.23          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 37       | 0.23          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 37       | 0.23          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 2        | 0.23          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 6        | 0.23          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 8        | 0.23          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 11       | 0.23          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 16       | 0.23          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 18       | 0.23          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 26       | 0.23          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 27       | 0.23          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 28       | 0.23          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 33       | 0.23          |
| (3,1963) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 37       | 0.23          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 1        | 0.23          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 1        | 0.23          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 1        | 0.23          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 5        | 0.23          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 5        | 0.23          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 5        | 0.23          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 6        | 0.23          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 6        | 0.23          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 6        | 0.23          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 8        | 0.23          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 8        | 0.23          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 8        | 0.23          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 14       | 0.23          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 14       | 0.23          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 14       | 0.23          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 17       | 0.23          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 17       | 0.23          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 17       | 0.23          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 20       | 0.23          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 20       | 0.23          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 20       | 0.23          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 23       | 0.23          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 23       | 0.23          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 23       | 0.23          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 25       | 0.23          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 25       | 0.23          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 25       | 0.23          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 27       | 0.23          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 27       | 0.23          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 27       | 0.23          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 30       | 0.23          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 30       | 0.23          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 30       | 0.23          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 34       | 0.23          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 34       | 0.23          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 34       | 0.23          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 35       | 0.23          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 35       | 0.23          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 35       | 0.23          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 3        | 0.23          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 6        | 0.23          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 8        | 0.23          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 12       | 0.23          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 13       | 0.23          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 14       | 0.23          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 17       | 0.23          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 19       | 0.23          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 20       | 0.23          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 21       | 0.23          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 24       | 0.23          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 25       | 0.23          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 26       | 0.23          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 27       | 0.23          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 28       | 0.23          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 29       | 0.23          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 30       | 0.23          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 31       | 0.23          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 32       | 0.23          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 33       | 0.23          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 36       | 0.23          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 37       | 0.23          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 38       | 0.23          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 39       | 0.23          |
| (3,1907) | 1:66:A:MET:HE1  | 1:43:A:TYR:H   | 15       | 0.23          |
| (3,1907) | 1:66:A:MET:HE2  | 1:43:A:TYR:H   | 15       | 0.23          |
| (3,1907) | 1:66:A:MET:HE3  | 1:43:A:TYR:H   | 15       | 0.23          |
| (3,1828) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA  | 38       | 0.23          |
| (3,1815) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA  | 38       | 0.23          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 2        | 0.23          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 6        | 0.23          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 8        | 0.23          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 11       | 0.23          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 16       | 0.23          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 18       | 0.23          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 26       | 0.23          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2 | 27       | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2  | 28       | 0.23          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2  | 33       | 0.23          |
| (3,1805) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2  | 37       | 0.23          |
| (3,1781) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H    | 15       | 0.23          |
| (3,1781) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H    | 19       | 0.23          |
| (3,1781) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H    | 20       | 0.23          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 2        | 0.23          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 2        | 0.23          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 2        | 0.23          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 13       | 0.23          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 13       | 0.23          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 13       | 0.23          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 17       | 0.23          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 17       | 0.23          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 17       | 0.23          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 11       | 0.23          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 11       | 0.23          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 11       | 0.23          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 11       | 0.23          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 11       | 0.23          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 11       | 0.23          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 11       | 0.23          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 11       | 0.23          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 11       | 0.23          |
| (3,1628) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2  | 24       | 0.23          |
| (3,1628) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2  | 24       | 0.23          |
| (3,1628) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2  | 24       | 0.23          |
| (3,1628) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2  | 27       | 0.23          |
| (3,1628) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2  | 27       | 0.23          |
| (3,1628) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2  | 27       | 0.23          |
| (3,1628) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2  | 28       | 0.23          |
| (3,1628) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2  | 28       | 0.23          |
| (3,1628) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2  | 28       | 0.23          |
| (3,1628) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2  | 35       | 0.23          |
| (3,1628) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2  | 35       | 0.23          |
| (3,1628) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2  | 35       | 0.23          |
| (3,1628) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2  | 40       | 0.23          |
| (3,1628) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2  | 40       | 0.23          |
| (3,1628) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2  | 40       | 0.23          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 26       | 0.23          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 26       | 0.23          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 26       | 0.23          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2 | 31       | 0.23          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 31       | 0.23          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 31       | 0.23          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2 | 36       | 0.23          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 36       | 0.23          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 36       | 0.23          |
| (3,1540) | 1:39:A:ILE:HD11 | 1:40:A:VAL:H   | 36       | 0.23          |
| (3,1540) | 1:39:A:ILE:HD12 | 1:40:A:VAL:H   | 36       | 0.23          |
| (3,1540) | 1:39:A:ILE:HD13 | 1:40:A:VAL:H   | 36       | 0.23          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 3        | 0.23          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 5        | 0.23          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 6        | 0.23          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 7        | 0.23          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 10       | 0.23          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 14       | 0.23          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 16       | 0.23          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 17       | 0.23          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 23       | 0.23          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 25       | 0.23          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 27       | 0.23          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 30       | 0.23          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 37       | 0.23          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 39       | 0.23          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 40       | 0.23          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 19       | 0.23          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 19       | 0.23          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 19       | 0.23          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 28       | 0.23          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 28       | 0.23          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 28       | 0.23          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H   | 11       | 0.23          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H   | 11       | 0.23          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H   | 11       | 0.23          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H   | 27       | 0.23          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H   | 27       | 0.23          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H   | 27       | 0.23          |
| (3,1400) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 1        | 0.23          |
| (3,1400) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 1        | 0.23          |
| (3,1400) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 1        | 0.23          |
| (3,1400) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 3        | 0.23          |
| (3,1400) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 3        | 0.23          |
| (3,1400) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 3        | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H    | 7        | 0.23          |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H    | 7        | 0.23          |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H    | 7        | 0.23          |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H    | 20       | 0.23          |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H    | 20       | 0.23          |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H    | 20       | 0.23          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 33       | 0.23          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 33       | 0.23          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 33       | 0.23          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 37       | 0.23          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 37       | 0.23          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 37       | 0.23          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 5        | 0.23          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 5        | 0.23          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 5        | 0.23          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 5        | 0.23          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 5        | 0.23          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 5        | 0.23          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 17       | 0.23          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 17       | 0.23          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 17       | 0.23          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 11       | 0.23          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 11       | 0.23          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 11       | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 1        | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 1        | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 1        | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 8        | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 8        | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 8        | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 13       | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 13       | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 13       | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 14       | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 14       | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 14       | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 15       | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 15       | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 15       | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 21       | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 21       | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 21       | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 22       | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 22       | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 22       | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 27       | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 27       | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 27       | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 28       | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 28       | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 28       | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 35       | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 35       | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 35       | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 40       | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 40       | 0.23          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 40       | 0.23          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 1        | 0.23          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 9        | 0.23          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 20       | 0.23          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 26       | 0.23          |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 9        | 0.23          |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 12       | 0.23          |
| (3,1188) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 6        | 0.23          |
| (3,1188) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 7        | 0.23          |
| (3,1188) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 10       | 0.23          |
| (3,1188) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 14       | 0.23          |
| (3,1188) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 17       | 0.23          |
| (3,1188) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 20       | 0.23          |
| (3,1188) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 22       | 0.23          |
| (3,1188) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 30       | 0.23          |
| (3,1188) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 31       | 0.23          |
| (3,1173) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 9        | 0.23          |
| (3,970)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 3        | 0.23          |
| (3,970)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 5        | 0.23          |
| (3,970)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 6        | 0.23          |
| (3,970)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 7        | 0.23          |
| (3,970)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 9        | 0.23          |
| (3,970)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 16       | 0.23          |
| (3,970)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 23       | 0.23          |
| (3,970)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 34       | 0.23          |
| (3,970)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 35       | 0.23          |
| (3,920)  | 1:37:A:ASP:H    | 1:36:A:ASP:HB2  | 40       | 0.23          |
| (3,919)  | 1:37:A:ASP:H    | 1:36:A:ASP:HB3  | 2        | 0.23          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,919) | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 6        | 0.23          |
| (3,919) | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 10       | 0.23          |
| (3,919) | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 19       | 0.23          |
| (3,919) | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 20       | 0.23          |
| (3,919) | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 28       | 0.23          |
| (3,919) | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 32       | 0.23          |
| (3,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3   | 28       | 0.23          |
| (3,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2   | 5        | 0.23          |
| (3,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2   | 9        | 0.23          |
| (3,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2   | 11       | 0.23          |
| (3,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2   | 15       | 0.23          |
| (3,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 30       | 0.23          |
| (3,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 36       | 0.23          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 6        | 0.23          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 6        | 0.23          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 6        | 0.23          |
| (3,826) | 1:17:A:GLN:H | 1:17:A:GLN:HG2  | 28       | 0.23          |
| (3,826) | 1:17:A:GLN:H | 1:17:A:GLN:HG2  | 29       | 0.23          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 12       | 0.23          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 12       | 0.23          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 12       | 0.23          |
| (3,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 8        | 0.23          |
| (3,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 14       | 0.23          |
| (3,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 21       | 0.23          |
| (3,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 22       | 0.23          |
| (3,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 23       | 0.23          |
| (3,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 24       | 0.23          |
| (3,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 25       | 0.23          |
| (3,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 26       | 0.23          |
| (3,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 27       | 0.23          |
| (3,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 30       | 0.23          |
| (3,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 31       | 0.23          |
| (3,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 32       | 0.23          |
| (3,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 33       | 0.23          |
| (3,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 34       | 0.23          |
| (3,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 35       | 0.23          |
| (3,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 38       | 0.23          |
| (3,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 39       | 0.23          |
| (3,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 40       | 0.23          |
| (3,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2  | 2        | 0.23          |
| (3,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2  | 3        | 0.23          |
| (3,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2  | 10       | 0.23          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (3,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2 | 24       | 0.23          |
| (3,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2 | 35       | 0.23          |
| (3,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3 | 1        | 0.23          |
| (3,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3 | 4        | 0.23          |
| (3,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3 | 6        | 0.23          |
| (3,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3 | 7        | 0.23          |
| (3,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3 | 12       | 0.23          |
| (3,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3 | 13       | 0.23          |
| (3,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3 | 19       | 0.23          |
| (3,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3 | 21       | 0.23          |
| (3,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3 | 24       | 0.23          |
| (3,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3 | 28       | 0.23          |
| (3,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3 | 29       | 0.23          |
| (3,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3 | 31       | 0.23          |
| (3,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3 | 32       | 0.23          |
| (3,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3 | 36       | 0.23          |
| (3,685) | 1:23:A:GLU:H  | 1:23:A:GLU:HG3 | 8        | 0.23          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3 | 17       | 0.23          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3 | 21       | 0.23          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3 | 26       | 0.23          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3 | 31       | 0.23          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3 | 32       | 0.23          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3 | 35       | 0.23          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3 | 36       | 0.23          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3 | 37       | 0.23          |
| (3,590) | 1:3:A:ASP:H   | 1:2:A:ILE:HA   | 15       | 0.23          |
| (3,590) | 1:3:A:ASP:H   | 1:2:A:ILE:HA   | 33       | 0.23          |
| (3,590) | 1:3:A:ASP:H   | 1:2:A:ILE:HA   | 35       | 0.23          |
| (3,556) | 1:47:A:THR:H  | 1:48:A:GLU:H   | 2        | 0.23          |
| (3,556) | 1:47:A:THR:H  | 1:48:A:GLU:H   | 39       | 0.23          |
| (3,546) | 1:71:A:VAL:H  | 1:24:A:HIS:HA  | 19       | 0.23          |
| (3,546) | 1:71:A:VAL:H  | 1:24:A:HIS:HA  | 23       | 0.23          |
| (3,546) | 1:71:A:VAL:H  | 1:24:A:HIS:HA  | 33       | 0.23          |
| (3,546) | 1:71:A:VAL:H  | 1:24:A:HIS:HA  | 36       | 0.23          |
| (3,546) | 1:71:A:VAL:H  | 1:24:A:HIS:HA  | 40       | 0.23          |
| (3,525) | 1:99:A:GLY:H  | 1:100:A:GLU:H  | 6        | 0.23          |
| (3,525) | 1:99:A:GLY:H  | 1:100:A:GLU:H  | 7        | 0.23          |
| (3,423) | 1:69:A:HIS:H  | 1:69:A:HIS:HD2 | 5        | 0.23          |
| (3,423) | 1:69:A:HIS:H  | 1:69:A:HIS:HD2 | 40       | 0.23          |
| (3,416) | 1:96:A:GLU:H  | 1:96:A:GLU:HB3 | 1        | 0.23          |
| (3,416) | 1:96:A:GLU:H  | 1:96:A:GLU:HB3 | 5        | 0.23          |
| (3,416) | 1:96:A:GLU:H  | 1:96:A:GLU:HB3 | 8        | 0.23          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3  | 15       | 0.23          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3  | 20       | 0.23          |
| (3,416) | 1:96:A:GLU:H | 1:96:A:GLU:HB3  | 33       | 0.23          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 28       | 0.23          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 36       | 0.23          |
| (3,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 28       | 0.23          |
| (3,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 29       | 0.23          |
| (3,365) | 1:18:A:ASN:H | 1:18:A:ASN:HB2  | 6        | 0.23          |
| (3,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 15       | 0.23          |
| (3,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 16       | 0.23          |
| (3,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 28       | 0.23          |
| (3,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 35       | 0.23          |
| (3,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 36       | 0.23          |
| (3,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 37       | 0.23          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 8        | 0.23          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 8        | 0.23          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 9        | 0.23          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 9        | 0.23          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 22       | 0.23          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 22       | 0.23          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 24       | 0.23          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 24       | 0.23          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 40       | 0.23          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 40       | 0.23          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 4        | 0.23          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 6        | 0.23          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 9        | 0.23          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 10       | 0.23          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 15       | 0.23          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 18       | 0.23          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 20       | 0.23          |
| (3,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 26       | 0.23          |
| (3,135) | 1:39:A:ILE:H | 1:39:A:ILE:HG13 | 11       | 0.23          |
| (3,135) | 1:39:A:ILE:H | 1:39:A:ILE:HG13 | 19       | 0.23          |
| (3,135) | 1:39:A:ILE:H | 1:39:A:ILE:HG13 | 36       | 0.23          |
| (3,131) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 1        | 0.23          |
| (3,131) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 3        | 0.23          |
| (3,131) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 4        | 0.23          |
| (3,131) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 5        | 0.23          |
| (3,131) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 6        | 0.23          |
| (3,131) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 8        | 0.23          |
| (3,131) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 9        | 0.23          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,131) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 10       | 0.23          |
| (3,131) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 12       | 0.23          |
| (3,131) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 14       | 0.23          |
| (3,131) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 15       | 0.23          |
| (3,131) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 17       | 0.23          |
| (3,131) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 18       | 0.23          |
| (3,131) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 20       | 0.23          |
| (3,131) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 22       | 0.23          |
| (3,131) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 23       | 0.23          |
| (3,131) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 25       | 0.23          |
| (3,131) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 26       | 0.23          |
| (3,131) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 27       | 0.23          |
| (3,131) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 29       | 0.23          |
| (3,131) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 30       | 0.23          |
| (3,131) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 31       | 0.23          |
| (3,131) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 32       | 0.23          |
| (3,131) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 33       | 0.23          |
| (3,131) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 34       | 0.23          |
| (3,131) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 35       | 0.23          |
| (3,131) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 37       | 0.23          |
| (3,131) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 39       | 0.23          |
| (3,131) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 40       | 0.23          |
| (3,74)  | 1:51:A:GLU:H | 1:50:A:THR:HG21 | 7        | 0.23          |
| (3,74)  | 1:51:A:GLU:H | 1:50:A:THR:HG22 | 7        | 0.23          |
| (3,74)  | 1:51:A:GLU:H | 1:50:A:THR:HG23 | 7        | 0.23          |
| (3,74)  | 1:51:A:GLU:H | 1:50:A:THR:HG21 | 13       | 0.23          |
| (3,74)  | 1:51:A:GLU:H | 1:50:A:THR:HG22 | 13       | 0.23          |
| (3,74)  | 1:51:A:GLU:H | 1:50:A:THR:HG23 | 13       | 0.23          |
| (3,74)  | 1:51:A:GLU:H | 1:50:A:THR:HG21 | 20       | 0.23          |
| (3,74)  | 1:51:A:GLU:H | 1:50:A:THR:HG22 | 20       | 0.23          |
| (3,74)  | 1:51:A:GLU:H | 1:50:A:THR:HG23 | 20       | 0.23          |
| (3,74)  | 1:51:A:GLU:H | 1:50:A:THR:HG21 | 21       | 0.23          |
| (3,74)  | 1:51:A:GLU:H | 1:50:A:THR:HG22 | 21       | 0.23          |
| (3,74)  | 1:51:A:GLU:H | 1:50:A:THR:HG23 | 21       | 0.23          |
| (3,74)  | 1:51:A:GLU:H | 1:50:A:THR:HG21 | 23       | 0.23          |
| (3,74)  | 1:51:A:GLU:H | 1:50:A:THR:HG22 | 23       | 0.23          |
| (3,74)  | 1:51:A:GLU:H | 1:50:A:THR:HG23 | 23       | 0.23          |
| (3,74)  | 1:51:A:GLU:H | 1:50:A:THR:HG21 | 25       | 0.23          |
| (3,74)  | 1:51:A:GLU:H | 1:50:A:THR:HG22 | 25       | 0.23          |
| (3,74)  | 1:51:A:GLU:H | 1:50:A:THR:HG23 | 25       | 0.23          |
| (3,74)  | 1:51:A:GLU:H | 1:50:A:THR:HG21 | 35       | 0.23          |
| (3,74)  | 1:51:A:GLU:H | 1:50:A:THR:HG22 | 35       | 0.23          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 35       | 0.23          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 36       | 0.23          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 36       | 0.23          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 36       | 0.23          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 38       | 0.23          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 38       | 0.23          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 38       | 0.23          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 17       | 0.23          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 17       | 0.23          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 28       | 0.23          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 28       | 0.23          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 31       | 0.23          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 31       | 0.23          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 2        | 0.23          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 2        | 0.23          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 2        | 0.23          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 2        | 0.23          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 2        | 0.23          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 2        | 0.23          |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 2        | 0.23          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 2        | 0.23          |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 5        | 0.23          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 5        | 0.23          |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 11       | 0.23          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 11       | 0.23          |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 13       | 0.23          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 13       | 0.23          |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 18       | 0.23          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 18       | 0.23          |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 21       | 0.23          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 21       | 0.23          |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 30       | 0.23          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 30       | 0.23          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 5        | 0.23          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 5        | 0.23          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 5        | 0.23          |
| (1,3048) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2  | 11       | 0.23          |
| (1,3048) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2  | 27       | 0.23          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 29       | 0.23          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H    | 4        | 0.23          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H    | 6        | 0.23          |
| (1,3046) | 1:57:A:PHE:HB3 | 1:57:A:PHE:H    | 7        | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3046) | 1:57:A:PHE:HB3  | 1:57:A:PHE:H    | 17       | 0.23          |
| (1,3046) | 1:57:A:PHE:HB3  | 1:57:A:PHE:H    | 19       | 0.23          |
| (1,3046) | 1:57:A:PHE:HB3  | 1:57:A:PHE:H    | 28       | 0.23          |
| (1,3046) | 1:57:A:PHE:HB3  | 1:57:A:PHE:H    | 34       | 0.23          |
| (1,3046) | 1:57:A:PHE:HB3  | 1:57:A:PHE:H    | 35       | 0.23          |
| (1,3046) | 1:57:A:PHE:HB3  | 1:57:A:PHE:H    | 36       | 0.23          |
| (1,3046) | 1:57:A:PHE:HB3  | 1:57:A:PHE:H    | 39       | 0.23          |
| (1,3004) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG21 | 20       | 0.23          |
| (1,3004) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG22 | 20       | 0.23          |
| (1,3004) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG23 | 20       | 0.23          |
| (1,3004) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG21 | 27       | 0.23          |
| (1,3004) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG22 | 27       | 0.23          |
| (1,3004) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG23 | 27       | 0.23          |
| (1,2931) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 5        | 0.23          |
| (1,2918) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 5        | 0.23          |
| (1,2918) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 27       | 0.23          |
| (1,2918) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 39       | 0.23          |
| (1,2916) | 1:22:A:SER:HB2  | 1:22:A:SER:H    | 7        | 0.23          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 1        | 0.23          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 2        | 0.23          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 3        | 0.23          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 4        | 0.23          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 5        | 0.23          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 6        | 0.23          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 7        | 0.23          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 8        | 0.23          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 9        | 0.23          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 10       | 0.23          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 11       | 0.23          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 14       | 0.23          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 15       | 0.23          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 16       | 0.23          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 18       | 0.23          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 21       | 0.23          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 23       | 0.23          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 25       | 0.23          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 26       | 0.23          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 27       | 0.23          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 29       | 0.23          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 31       | 0.23          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 32       | 0.23          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 33       | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 35       | 0.23          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 36       | 0.23          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 37       | 0.23          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 38       | 0.23          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 39       | 0.23          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 40       | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 1        | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 2        | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 3        | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 4        | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 5        | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 6        | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 7        | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 8        | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 9        | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 10       | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 11       | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 14       | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 15       | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 16       | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 18       | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 21       | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 23       | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 25       | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 26       | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 27       | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 29       | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 31       | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 32       | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 33       | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 35       | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 36       | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 37       | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 38       | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 39       | 0.23          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 40       | 0.23          |
| (1,2718) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 2        | 0.23          |
| (1,2718) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 3        | 0.23          |
| (1,2718) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 5        | 0.23          |
| (1,2718) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 6        | 0.23          |
| (1,2718) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 8        | 0.23          |
| (1,2718) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 9        | 0.23          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,2718) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 10       | 0.23          |
| (1,2718) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 11       | 0.23          |
| (1,2718) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 12       | 0.23          |
| (1,2718) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 18       | 0.23          |
| (1,2718) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 21       | 0.23          |
| (1,2718) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 24       | 0.23          |
| (1,2718) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 25       | 0.23          |
| (1,2718) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 27       | 0.23          |
| (1,2718) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 29       | 0.23          |
| (1,2718) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 30       | 0.23          |
| (1,2718) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 31       | 0.23          |
| (1,2718) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 34       | 0.23          |
| (1,2718) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 35       | 0.23          |
| (1,2718) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 36       | 0.23          |
| (1,2718) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 37       | 0.23          |
| (1,2718) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 38       | 0.23          |
| (1,2718) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 39       | 0.23          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 1        | 0.23          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 2        | 0.23          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 3        | 0.23          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 4        | 0.23          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 5        | 0.23          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 9        | 0.23          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 11       | 0.23          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 14       | 0.23          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 15       | 0.23          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 16       | 0.23          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 17       | 0.23          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 20       | 0.23          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 21       | 0.23          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 22       | 0.23          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 24       | 0.23          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 25       | 0.23          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 26       | 0.23          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 27       | 0.23          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 30       | 0.23          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 32       | 0.23          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 34       | 0.23          |
| (1,2693) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 38       | 0.23          |
| (1,2672) | 1:25:A:GLN:HG3 | 1:22:A:SER:HB2 | 7        | 0.23          |
| (1,2668) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 5        | 0.23          |
| (1,2668) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 9        | 0.23          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,2668) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA   | 10       | 0.23          |
| (1,2649) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 28       | 0.23          |
| (1,2649) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 29       | 0.23          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3   | 3        | 0.23          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3   | 5        | 0.23          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3   | 8        | 0.23          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3   | 19       | 0.23          |
| (1,2598) | 1:36:A:ASP:HB2 | 1:37:A:ASP:H    | 40       | 0.23          |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H    | 2        | 0.23          |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H    | 6        | 0.23          |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H    | 10       | 0.23          |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H    | 19       | 0.23          |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H    | 20       | 0.23          |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H    | 28       | 0.23          |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H    | 32       | 0.23          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA   | 23       | 0.23          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA   | 36       | 0.23          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA   | 37       | 0.23          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA   | 40       | 0.23          |
| (1,2534) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3  | 7        | 0.23          |
| (1,2534) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3  | 8        | 0.23          |
| (1,2534) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3  | 12       | 0.23          |
| (1,2534) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3  | 13       | 0.23          |
| (1,2467) | 1:4:A:PRO:HB2  | 1:4:A:PRO:HD2   | 17       | 0.23          |
| (1,2402) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ   | 34       | 0.23          |
| (1,2402) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ   | 34       | 0.23          |
| (1,2402) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ   | 34       | 0.23          |
| (1,2324) | 1:80:A:SER:HB2 | 1:94:A:THR:HG21 | 28       | 0.23          |
| (1,2324) | 1:80:A:SER:HB2 | 1:94:A:THR:HG22 | 28       | 0.23          |
| (1,2324) | 1:80:A:SER:HB2 | 1:94:A:THR:HG23 | 28       | 0.23          |
| (1,2322) | 1:80:A:SER:HB2 | 1:81:A:VAL:H    | 1        | 0.23          |
| (1,2322) | 1:80:A:SER:HB2 | 1:81:A:VAL:H    | 18       | 0.23          |
| (1,2322) | 1:80:A:SER:HB2 | 1:81:A:VAL:H    | 20       | 0.23          |
| (1,2322) | 1:80:A:SER:HB2 | 1:81:A:VAL:H    | 23       | 0.23          |
| (1,2322) | 1:80:A:SER:HB2 | 1:81:A:VAL:H    | 25       | 0.23          |
| (1,2322) | 1:80:A:SER:HB2 | 1:81:A:VAL:H    | 30       | 0.23          |
| (1,2322) | 1:80:A:SER:HB2 | 1:81:A:VAL:H    | 32       | 0.23          |
| (1,2322) | 1:80:A:SER:HB2 | 1:81:A:VAL:H    | 36       | 0.23          |
| (1,2286) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H    | 6        | 0.23          |
| (1,2250) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 25       | 0.23          |
| (1,2250) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 25       | 0.23          |
| (1,2250) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 34       | 0.23          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,2250) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2 | 34       | 0.23          |
| (1,2250) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1 | 38       | 0.23          |
| (1,2250) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2 | 38       | 0.23          |
| (1,2250) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1 | 40       | 0.23          |
| (1,2250) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2 | 40       | 0.23          |
| (1,2170) | 1:43:A:TYR:HA  | 1:80:A:SER:H   | 2        | 0.23          |
| (1,2170) | 1:43:A:TYR:HA  | 1:80:A:SER:H   | 4        | 0.23          |
| (1,2170) | 1:43:A:TYR:HA  | 1:80:A:SER:H   | 16       | 0.23          |
| (1,2170) | 1:43:A:TYR:HA  | 1:80:A:SER:H   | 18       | 0.23          |
| (1,2170) | 1:43:A:TYR:HA  | 1:80:A:SER:H   | 19       | 0.23          |
| (1,2170) | 1:43:A:TYR:HA  | 1:80:A:SER:H   | 37       | 0.23          |
| (1,2170) | 1:43:A:TYR:HA  | 1:80:A:SER:H   | 39       | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 1        | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 2        | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 3        | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 4        | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 5        | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 6        | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 7        | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 8        | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 9        | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 10       | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 11       | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 12       | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 13       | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 14       | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 15       | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 17       | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 18       | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 19       | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 20       | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 21       | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 22       | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 23       | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 24       | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 25       | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 26       | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 27       | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 28       | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 29       | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 30       | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2  | 1:5:A:PHE:HB3  | 31       | 0.23          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (1,2151) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 32       | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 34       | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 35       | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 36       | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 37       | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 38       | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 39       | 0.23          |
| (1,2151) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 40       | 0.23          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 8        | 0.23          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 8        | 0.23          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 8        | 0.23          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 9        | 0.23          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 9        | 0.23          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 9        | 0.23          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 16       | 0.23          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 16       | 0.23          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 16       | 0.23          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 18       | 0.23          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 18       | 0.23          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 18       | 0.23          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 20       | 0.23          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 20       | 0.23          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 20       | 0.23          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 27       | 0.23          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 27       | 0.23          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 27       | 0.23          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 28       | 0.23          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 28       | 0.23          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 28       | 0.23          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 31       | 0.23          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 31       | 0.23          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 31       | 0.23          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 32       | 0.23          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 32       | 0.23          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 32       | 0.23          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 38       | 0.23          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 38       | 0.23          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 38       | 0.23          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 40       | 0.23          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 40       | 0.23          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 40       | 0.23          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA | 9        | 0.23          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 9        | 0.23          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 9        | 0.23          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 14       | 0.23          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 14       | 0.23          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 14       | 0.23          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 19       | 0.23          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 19       | 0.23          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 19       | 0.23          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 23       | 0.23          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 23       | 0.23          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 23       | 0.23          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 25       | 0.23          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 25       | 0.23          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 25       | 0.23          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 26       | 0.23          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 26       | 0.23          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 26       | 0.23          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 27       | 0.23          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 27       | 0.23          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 27       | 0.23          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 29       | 0.23          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 29       | 0.23          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 29       | 0.23          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 30       | 0.23          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 30       | 0.23          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 30       | 0.23          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 33       | 0.23          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 33       | 0.23          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 33       | 0.23          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 13       | 0.23          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 13       | 0.23          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 13       | 0.23          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 17       | 0.23          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 17       | 0.23          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 17       | 0.23          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 17       | 0.23          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 17       | 0.23          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 17       | 0.23          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 18       | 0.23          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 18       | 0.23          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 18       | 0.23          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 18       | 0.23          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 18       | 0.23          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 18       | 0.23          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 22       | 0.23          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 22       | 0.23          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 22       | 0.23          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 22       | 0.23          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 22       | 0.23          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 22       | 0.23          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 27       | 0.23          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 27       | 0.23          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 27       | 0.23          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 27       | 0.23          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 27       | 0.23          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 27       | 0.23          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 32       | 0.23          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 32       | 0.23          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 32       | 0.23          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 32       | 0.23          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 32       | 0.23          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 32       | 0.23          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 36       | 0.23          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 36       | 0.23          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 36       | 0.23          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 36       | 0.23          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 36       | 0.23          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 36       | 0.23          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 14       | 0.23          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 14       | 0.23          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 14       | 0.23          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 29       | 0.23          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 29       | 0.23          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 29       | 0.23          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 40       | 0.23          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 40       | 0.23          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 40       | 0.23          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 13       | 0.23          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 13       | 0.23          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 13       | 0.23          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 18       | 0.23          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 18       | 0.23          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 18       | 0.23          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 25       | 0.23          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 25       | 0.23          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 25       | 0.23          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 27       | 0.23          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 27       | 0.23          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 27       | 0.23          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 30       | 0.23          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 30       | 0.23          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 30       | 0.23          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 34       | 0.23          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 34       | 0.23          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 34       | 0.23          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 36       | 0.23          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 36       | 0.23          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 36       | 0.23          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 37       | 0.23          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 37       | 0.23          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 37       | 0.23          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 2        | 0.23          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 6        | 0.23          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 8        | 0.23          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 11       | 0.23          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 16       | 0.23          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 18       | 0.23          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 26       | 0.23          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 27       | 0.23          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 28       | 0.23          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 33       | 0.23          |
| (1,1960) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 37       | 0.23          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 1        | 0.23          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 1        | 0.23          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 1        | 0.23          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 5        | 0.23          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 5        | 0.23          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 5        | 0.23          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 6        | 0.23          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 6        | 0.23          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 6        | 0.23          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 8        | 0.23          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 8        | 0.23          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 8        | 0.23          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 14       | 0.23          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 14       | 0.23          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 14       | 0.23          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 17       | 0.23          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 17       | 0.23          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 17       | 0.23          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 20       | 0.23          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 20       | 0.23          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 20       | 0.23          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 23       | 0.23          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 23       | 0.23          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 23       | 0.23          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 25       | 0.23          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 25       | 0.23          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 25       | 0.23          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 27       | 0.23          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 27       | 0.23          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 27       | 0.23          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 30       | 0.23          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 30       | 0.23          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 30       | 0.23          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 34       | 0.23          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 34       | 0.23          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 34       | 0.23          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 35       | 0.23          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 35       | 0.23          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 35       | 0.23          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 3        | 0.23          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 6        | 0.23          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 8        | 0.23          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 12       | 0.23          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 13       | 0.23          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 14       | 0.23          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 17       | 0.23          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 19       | 0.23          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 20       | 0.23          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 21       | 0.23          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 24       | 0.23          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 25       | 0.23          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 26       | 0.23          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 27       | 0.23          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 28       | 0.23          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 29       | 0.23          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 30       | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2  | 31       | 0.23          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2  | 32       | 0.23          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2  | 33       | 0.23          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2  | 36       | 0.23          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2  | 37       | 0.23          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2  | 38       | 0.23          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2  | 39       | 0.23          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 9        | 0.23          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 9        | 0.23          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 9        | 0.23          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 9        | 0.23          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 9        | 0.23          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 9        | 0.23          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 9        | 0.23          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 9        | 0.23          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 9        | 0.23          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 31       | 0.23          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 31       | 0.23          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 31       | 0.23          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 31       | 0.23          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 31       | 0.23          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 31       | 0.23          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 31       | 0.23          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 31       | 0.23          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 31       | 0.23          |
| (1,1904) | 1:66:A:MET:HE1  | 1:43:A:TYR:H    | 15       | 0.23          |
| (1,1904) | 1:66:A:MET:HE2  | 1:43:A:TYR:H    | 15       | 0.23          |
| (1,1904) | 1:66:A:MET:HE3  | 1:43:A:TYR:H    | 15       | 0.23          |
| (1,1825) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 38       | 0.23          |
| (1,1812) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 38       | 0.23          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2  | 2        | 0.23          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2  | 6        | 0.23          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2  | 8        | 0.23          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2  | 11       | 0.23          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2  | 16       | 0.23          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2  | 18       | 0.23          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2  | 26       | 0.23          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2  | 27       | 0.23          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2  | 28       | 0.23          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2  | 33       | 0.23          |
| (1,1802) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HD2  | 37       | 0.23          |
| (1,1778) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H    | 15       | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1778) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H    | 19       | 0.23          |
| (1,1778) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H    | 20       | 0.23          |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 2        | 0.23          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 2        | 0.23          |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 2        | 0.23          |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 13       | 0.23          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 13       | 0.23          |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 13       | 0.23          |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 17       | 0.23          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 17       | 0.23          |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 17       | 0.23          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 11       | 0.23          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 11       | 0.23          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 11       | 0.23          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 11       | 0.23          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 11       | 0.23          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 11       | 0.23          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 11       | 0.23          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 11       | 0.23          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 11       | 0.23          |
| (1,1624) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2  | 24       | 0.23          |
| (1,1624) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2  | 24       | 0.23          |
| (1,1624) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2  | 24       | 0.23          |
| (1,1624) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2  | 27       | 0.23          |
| (1,1624) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2  | 27       | 0.23          |
| (1,1624) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2  | 27       | 0.23          |
| (1,1624) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2  | 28       | 0.23          |
| (1,1624) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2  | 28       | 0.23          |
| (1,1624) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2  | 28       | 0.23          |
| (1,1624) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2  | 35       | 0.23          |
| (1,1624) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2  | 35       | 0.23          |
| (1,1624) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2  | 35       | 0.23          |
| (1,1624) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2  | 40       | 0.23          |
| (1,1624) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2  | 40       | 0.23          |
| (1,1624) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2  | 40       | 0.23          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 26       | 0.23          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 26       | 0.23          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 26       | 0.23          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 31       | 0.23          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 31       | 0.23          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 31       | 0.23          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 36       | 0.23          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 36       | 0.23          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 36       | 0.23          |
| (1,1536) | 1:39:A:ILE:HD11 | 1:40:A:VAL:H   | 36       | 0.23          |
| (1,1536) | 1:39:A:ILE:HD12 | 1:40:A:VAL:H   | 36       | 0.23          |
| (1,1536) | 1:39:A:ILE:HD13 | 1:40:A:VAL:H   | 36       | 0.23          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 3        | 0.23          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 5        | 0.23          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 6        | 0.23          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 7        | 0.23          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 10       | 0.23          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 14       | 0.23          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 16       | 0.23          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 17       | 0.23          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 23       | 0.23          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 25       | 0.23          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 27       | 0.23          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 30       | 0.23          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 37       | 0.23          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 39       | 0.23          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 40       | 0.23          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 19       | 0.23          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 19       | 0.23          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 19       | 0.23          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 28       | 0.23          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 28       | 0.23          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 28       | 0.23          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H   | 11       | 0.23          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H   | 11       | 0.23          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H   | 11       | 0.23          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H   | 27       | 0.23          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H   | 27       | 0.23          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H   | 27       | 0.23          |
| (1,1396) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 1        | 0.23          |
| (1,1396) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 1        | 0.23          |
| (1,1396) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 1        | 0.23          |
| (1,1396) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 3        | 0.23          |
| (1,1396) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 3        | 0.23          |
| (1,1396) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 3        | 0.23          |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 7        | 0.23          |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 7        | 0.23          |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 7        | 0.23          |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 20       | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H    | 20       | 0.23          |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H    | 20       | 0.23          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 33       | 0.23          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 33       | 0.23          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 33       | 0.23          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 37       | 0.23          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 37       | 0.23          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 37       | 0.23          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 5        | 0.23          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 5        | 0.23          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 5        | 0.23          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 5        | 0.23          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 5        | 0.23          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 5        | 0.23          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 17       | 0.23          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 17       | 0.23          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 17       | 0.23          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 11       | 0.23          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 11       | 0.23          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 11       | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 1        | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 1        | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 1        | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 8        | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 8        | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 8        | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 13       | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 13       | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 13       | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 14       | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 14       | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 14       | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 15       | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 15       | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 15       | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 21       | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 21       | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 21       | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 22       | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 22       | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 22       | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 27       | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 27       | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 27       | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 28       | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 28       | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 28       | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 35       | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 35       | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 35       | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 40       | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 40       | 0.23          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 40       | 0.23          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 1        | 0.23          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 9        | 0.23          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 20       | 0.23          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 26       | 0.23          |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 9        | 0.23          |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 12       | 0.23          |
| (1,1184) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 6        | 0.23          |
| (1,1184) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 7        | 0.23          |
| (1,1184) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 10       | 0.23          |
| (1,1184) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 14       | 0.23          |
| (1,1184) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 17       | 0.23          |
| (1,1184) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 20       | 0.23          |
| (1,1184) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 22       | 0.23          |
| (1,1184) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 30       | 0.23          |
| (1,1184) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 31       | 0.23          |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 9        | 0.23          |
| (1,969)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 3        | 0.23          |
| (1,969)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 5        | 0.23          |
| (1,969)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 6        | 0.23          |
| (1,969)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 7        | 0.23          |
| (1,969)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 9        | 0.23          |
| (1,969)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 16       | 0.23          |
| (1,969)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 23       | 0.23          |
| (1,969)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 34       | 0.23          |
| (1,969)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 35       | 0.23          |
| (1,919)  | 1:37:A:ASP:H    | 1:36:A:ASP:HB2  | 40       | 0.23          |
| (1,918)  | 1:37:A:ASP:H    | 1:36:A:ASP:HB3  | 2        | 0.23          |
| (1,918)  | 1:37:A:ASP:H    | 1:36:A:ASP:HB3  | 6        | 0.23          |
| (1,918)  | 1:37:A:ASP:H    | 1:36:A:ASP:HB3  | 10       | 0.23          |
| (1,918)  | 1:37:A:ASP:H    | 1:36:A:ASP:HB3  | 19       | 0.23          |
| (1,918)  | 1:37:A:ASP:H    | 1:36:A:ASP:HB3  | 20       | 0.23          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,918) | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 28       | 0.23          |
| (1,918) | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 32       | 0.23          |
| (1,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3   | 28       | 0.23          |
| (1,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2   | 5        | 0.23          |
| (1,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2   | 9        | 0.23          |
| (1,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2   | 11       | 0.23          |
| (1,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2   | 15       | 0.23          |
| (1,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 30       | 0.23          |
| (1,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 36       | 0.23          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 6        | 0.23          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 6        | 0.23          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 6        | 0.23          |
| (1,826) | 1:17:A:GLN:H | 1:17:A:GLN:HG2  | 28       | 0.23          |
| (1,826) | 1:17:A:GLN:H | 1:17:A:GLN:HG2  | 29       | 0.23          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 12       | 0.23          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 12       | 0.23          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 12       | 0.23          |
| (1,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 8        | 0.23          |
| (1,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 14       | 0.23          |
| (1,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 21       | 0.23          |
| (1,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 22       | 0.23          |
| (1,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 23       | 0.23          |
| (1,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 24       | 0.23          |
| (1,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 25       | 0.23          |
| (1,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 26       | 0.23          |
| (1,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 27       | 0.23          |
| (1,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 30       | 0.23          |
| (1,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 31       | 0.23          |
| (1,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 32       | 0.23          |
| (1,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 33       | 0.23          |
| (1,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 34       | 0.23          |
| (1,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 35       | 0.23          |
| (1,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 38       | 0.23          |
| (1,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 39       | 0.23          |
| (1,768) | 1:75:A:ASP:H | 1:75:A:ASP:HB3  | 40       | 0.23          |
| (1,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2  | 2        | 0.23          |
| (1,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2  | 3        | 0.23          |
| (1,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2  | 10       | 0.23          |
| (1,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2  | 24       | 0.23          |
| (1,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2  | 35       | 0.23          |
| (1,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3  | 1        | 0.23          |
| (1,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3  | 4        | 0.23          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3 | 6        | 0.23          |
| (1,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3 | 7        | 0.23          |
| (1,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3 | 12       | 0.23          |
| (1,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3 | 13       | 0.23          |
| (1,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3 | 19       | 0.23          |
| (1,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3 | 21       | 0.23          |
| (1,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3 | 24       | 0.23          |
| (1,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3 | 28       | 0.23          |
| (1,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3 | 29       | 0.23          |
| (1,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3 | 31       | 0.23          |
| (1,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3 | 32       | 0.23          |
| (1,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3 | 36       | 0.23          |
| (1,685) | 1:23:A:GLU:H  | 1:23:A:GLU:HG3 | 8        | 0.23          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3 | 17       | 0.23          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3 | 21       | 0.23          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3 | 26       | 0.23          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3 | 31       | 0.23          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3 | 32       | 0.23          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3 | 35       | 0.23          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3 | 36       | 0.23          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3 | 37       | 0.23          |
| (1,590) | 1:3:A:ASP:H   | 1:2:A:ILE:HA   | 15       | 0.23          |
| (1,590) | 1:3:A:ASP:H   | 1:2:A:ILE:HA   | 33       | 0.23          |
| (1,590) | 1:3:A:ASP:H   | 1:2:A:ILE:HA   | 35       | 0.23          |
| (1,556) | 1:47:A:THR:H  | 1:48:A:GLU:H   | 2        | 0.23          |
| (1,556) | 1:47:A:THR:H  | 1:48:A:GLU:H   | 39       | 0.23          |
| (1,546) | 1:71:A:VAL:H  | 1:24:A:HIS:HA  | 19       | 0.23          |
| (1,546) | 1:71:A:VAL:H  | 1:24:A:HIS:HA  | 23       | 0.23          |
| (1,546) | 1:71:A:VAL:H  | 1:24:A:HIS:HA  | 33       | 0.23          |
| (1,546) | 1:71:A:VAL:H  | 1:24:A:HIS:HA  | 36       | 0.23          |
| (1,546) | 1:71:A:VAL:H  | 1:24:A:HIS:HA  | 40       | 0.23          |
| (1,525) | 1:99:A:GLY:H  | 1:100:A:GLU:H  | 6        | 0.23          |
| (1,525) | 1:99:A:GLY:H  | 1:100:A:GLU:H  | 7        | 0.23          |
| (1,423) | 1:69:A:HIS:H  | 1:69:A:HIS:HD2 | 5        | 0.23          |
| (1,423) | 1:69:A:HIS:H  | 1:69:A:HIS:HD2 | 40       | 0.23          |
| (1,416) | 1:96:A:GLU:H  | 1:96:A:GLU:HB3 | 1        | 0.23          |
| (1,416) | 1:96:A:GLU:H  | 1:96:A:GLU:HB3 | 5        | 0.23          |
| (1,416) | 1:96:A:GLU:H  | 1:96:A:GLU:HB3 | 8        | 0.23          |
| (1,416) | 1:96:A:GLU:H  | 1:96:A:GLU:HB3 | 15       | 0.23          |
| (1,416) | 1:96:A:GLU:H  | 1:96:A:GLU:HB3 | 20       | 0.23          |
| (1,416) | 1:96:A:GLU:H  | 1:96:A:GLU:HB3 | 33       | 0.23          |
| (1,394) | 1:77:A:GLY:H  | 1:97:A:LEU:HA  | 28       | 0.23          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 36       | 0.23          |
| (1,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 28       | 0.23          |
| (1,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 29       | 0.23          |
| (1,365) | 1:18:A:ASN:H | 1:18:A:ASN:HB2  | 6        | 0.23          |
| (1,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 15       | 0.23          |
| (1,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 16       | 0.23          |
| (1,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 28       | 0.23          |
| (1,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 35       | 0.23          |
| (1,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 36       | 0.23          |
| (1,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 37       | 0.23          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 8        | 0.23          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 8        | 0.23          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 9        | 0.23          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 9        | 0.23          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 22       | 0.23          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 22       | 0.23          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 24       | 0.23          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 24       | 0.23          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 40       | 0.23          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 40       | 0.23          |
| (1,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 4        | 0.23          |
| (1,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 6        | 0.23          |
| (1,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 9        | 0.23          |
| (1,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 10       | 0.23          |
| (1,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 15       | 0.23          |
| (1,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 18       | 0.23          |
| (1,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 20       | 0.23          |
| (1,169) | 1:10:A:ILE:H | 1:10:A:ILE:HG12 | 26       | 0.23          |
| (1,149) | 1:45:A:GLY:H | 1:46:A:PRO:HD3  | 10       | 0.23          |
| (1,149) | 1:45:A:GLY:H | 1:46:A:PRO:HD3  | 19       | 0.23          |
| (1,133) | 1:39:A:ILE:H | 1:39:A:ILE:HG13 | 11       | 0.23          |
| (1,133) | 1:39:A:ILE:H | 1:39:A:ILE:HG13 | 19       | 0.23          |
| (1,133) | 1:39:A:ILE:H | 1:39:A:ILE:HG13 | 36       | 0.23          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 1        | 0.23          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 3        | 0.23          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 4        | 0.23          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 5        | 0.23          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 6        | 0.23          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 8        | 0.23          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 9        | 0.23          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 10       | 0.23          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 12       | 0.23          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 14       | 0.23          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 15       | 0.23          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 17       | 0.23          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 18       | 0.23          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 20       | 0.23          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 22       | 0.23          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 23       | 0.23          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 25       | 0.23          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 26       | 0.23          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 27       | 0.23          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 29       | 0.23          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 30       | 0.23          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 31       | 0.23          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 32       | 0.23          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 33       | 0.23          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 34       | 0.23          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 35       | 0.23          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 37       | 0.23          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 39       | 0.23          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 40       | 0.23          |
| (1,72)  | 1:51:A:GLU:H | 1:50:A:THR:HG21 | 7        | 0.23          |
| (1,72)  | 1:51:A:GLU:H | 1:50:A:THR:HG22 | 7        | 0.23          |
| (1,72)  | 1:51:A:GLU:H | 1:50:A:THR:HG23 | 7        | 0.23          |
| (1,72)  | 1:51:A:GLU:H | 1:50:A:THR:HG21 | 13       | 0.23          |
| (1,72)  | 1:51:A:GLU:H | 1:50:A:THR:HG22 | 13       | 0.23          |
| (1,72)  | 1:51:A:GLU:H | 1:50:A:THR:HG23 | 13       | 0.23          |
| (1,72)  | 1:51:A:GLU:H | 1:50:A:THR:HG21 | 20       | 0.23          |
| (1,72)  | 1:51:A:GLU:H | 1:50:A:THR:HG22 | 20       | 0.23          |
| (1,72)  | 1:51:A:GLU:H | 1:50:A:THR:HG23 | 20       | 0.23          |
| (1,72)  | 1:51:A:GLU:H | 1:50:A:THR:HG21 | 21       | 0.23          |
| (1,72)  | 1:51:A:GLU:H | 1:50:A:THR:HG22 | 21       | 0.23          |
| (1,72)  | 1:51:A:GLU:H | 1:50:A:THR:HG23 | 21       | 0.23          |
| (1,72)  | 1:51:A:GLU:H | 1:50:A:THR:HG21 | 23       | 0.23          |
| (1,72)  | 1:51:A:GLU:H | 1:50:A:THR:HG22 | 23       | 0.23          |
| (1,72)  | 1:51:A:GLU:H | 1:50:A:THR:HG23 | 23       | 0.23          |
| (1,72)  | 1:51:A:GLU:H | 1:50:A:THR:HG21 | 25       | 0.23          |
| (1,72)  | 1:51:A:GLU:H | 1:50:A:THR:HG22 | 25       | 0.23          |
| (1,72)  | 1:51:A:GLU:H | 1:50:A:THR:HG23 | 25       | 0.23          |
| (1,72)  | 1:51:A:GLU:H | 1:50:A:THR:HG21 | 35       | 0.23          |
| (1,72)  | 1:51:A:GLU:H | 1:50:A:THR:HG22 | 35       | 0.23          |
| (1,72)  | 1:51:A:GLU:H | 1:50:A:THR:HG23 | 35       | 0.23          |
| (1,72)  | 1:51:A:GLU:H | 1:50:A:THR:HG21 | 36       | 0.23          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 36       | 0.23          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 36       | 0.23          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 38       | 0.23          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 38       | 0.23          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 38       | 0.23          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 13       | 0.22          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 13       | 0.22          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 15       | 0.22          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 15       | 0.22          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 25       | 0.22          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 25       | 0.22          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 29       | 0.22          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 29       | 0.22          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 36       | 0.22          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 36       | 0.22          |
| (3,3217) | 1:69:A:HIS:HE1 | 1:67:A:THR:HB   | 17       | 0.22          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 7        | 0.22          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 7        | 0.22          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 17       | 0.22          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 18       | 0.22          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 20       | 0.22          |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2  | 34       | 0.22          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2  | 34       | 0.22          |
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 4        | 0.22          |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 4        | 0.22          |
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 17       | 0.22          |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 17       | 0.22          |
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 20       | 0.22          |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 20       | 0.22          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 34       | 0.22          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 34       | 0.22          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 34       | 0.22          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 34       | 0.22          |
| (3,3056) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2  | 37       | 0.22          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 24       | 0.22          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 13       | 0.22          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 13       | 0.22          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 13       | 0.22          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 34       | 0.22          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 34       | 0.22          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 34       | 0.22          |
| (3,3004) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 1        | 0.22          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,2976) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3 | 1        | 0.22          |
| (3,2976) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3 | 3        | 0.22          |
| (3,2976) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3 | 4        | 0.22          |
| (3,2976) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3 | 5        | 0.22          |
| (3,2976) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3 | 6        | 0.22          |
| (3,2976) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3 | 7        | 0.22          |
| (3,2976) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3 | 10       | 0.22          |
| (3,2976) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3 | 11       | 0.22          |
| (3,2976) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3 | 12       | 0.22          |
| (3,2976) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3 | 13       | 0.22          |
| (3,2976) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3 | 14       | 0.22          |
| (3,2976) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3 | 15       | 0.22          |
| (3,2976) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3 | 18       | 0.22          |
| (3,2976) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3 | 23       | 0.22          |
| (3,2976) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3 | 25       | 0.22          |
| (3,2976) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3 | 26       | 0.22          |
| (3,2976) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3 | 27       | 0.22          |
| (3,2976) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3 | 29       | 0.22          |
| (3,2976) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3 | 30       | 0.22          |
| (3,2976) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3 | 31       | 0.22          |
| (3,2976) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3 | 32       | 0.22          |
| (3,2976) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3 | 33       | 0.22          |
| (3,2976) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3 | 34       | 0.22          |
| (3,2976) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3 | 36       | 0.22          |
| (3,2976) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3 | 37       | 0.22          |
| (3,2976) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3 | 38       | 0.22          |
| (3,2969) | 1:44:A:LYS:HE2 | 1:44:A:LYS:HG2 | 2        | 0.22          |
| (3,2969) | 1:44:A:LYS:HE2 | 1:44:A:LYS:HG2 | 20       | 0.22          |
| (3,2925) | 1:22:A:SER:HB2 | 1:25:A:GLN:H   | 3        | 0.22          |
| (3,2925) | 1:22:A:SER:HB2 | 1:25:A:GLN:H   | 16       | 0.22          |
| (3,2864) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 1        | 0.22          |
| (3,2864) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 9        | 0.22          |
| (3,2864) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 10       | 0.22          |
| (3,2864) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 13       | 0.22          |
| (3,2864) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 14       | 0.22          |
| (3,2864) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 18       | 0.22          |
| (3,2864) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 35       | 0.22          |
| (3,2864) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 38       | 0.22          |
| (3,2809) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2 | 28       | 0.22          |
| (3,2808) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HG2 | 2        | 0.22          |
| (3,2808) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HG2 | 5        | 0.22          |
| (3,2808) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HG2 | 8        | 0.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2808) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HG2  | 9        | 0.22          |
| (3,2808) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HG2  | 16       | 0.22          |
| (3,2808) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HG2  | 25       | 0.22          |
| (3,2808) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HG2  | 30       | 0.22          |
| (3,2808) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HG2  | 33       | 0.22          |
| (3,2808) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HG2  | 37       | 0.22          |
| (3,2803) | 1:15:A:ARG:HG3  | 1:15:A:ARG:HB3  | 2        | 0.22          |
| (3,2803) | 1:15:A:ARG:HG3  | 1:15:A:ARG:HB3  | 5        | 0.22          |
| (3,2803) | 1:15:A:ARG:HG3  | 1:15:A:ARG:HB3  | 8        | 0.22          |
| (3,2803) | 1:15:A:ARG:HG3  | 1:15:A:ARG:HB3  | 11       | 0.22          |
| (3,2803) | 1:15:A:ARG:HG3  | 1:15:A:ARG:HB3  | 30       | 0.22          |
| (3,2803) | 1:15:A:ARG:HG3  | 1:15:A:ARG:HB3  | 31       | 0.22          |
| (3,2803) | 1:15:A:ARG:HG3  | 1:15:A:ARG:HB3  | 33       | 0.22          |
| (3,2803) | 1:15:A:ARG:HG3  | 1:15:A:ARG:HB3  | 38       | 0.22          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 12       | 0.22          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 13       | 0.22          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 17       | 0.22          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 19       | 0.22          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 20       | 0.22          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 22       | 0.22          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 24       | 0.22          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 28       | 0.22          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 30       | 0.22          |
| (3,2787) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 34       | 0.22          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 12       | 0.22          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 13       | 0.22          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 17       | 0.22          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 19       | 0.22          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 20       | 0.22          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 22       | 0.22          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 24       | 0.22          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 28       | 0.22          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 30       | 0.22          |
| (3,2786) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 34       | 0.22          |
| (3,2761) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 24       | 0.22          |
| (3,2761) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 25       | 0.22          |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 4        | 0.22          |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 7        | 0.22          |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 17       | 0.22          |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 23       | 0.22          |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 28       | 0.22          |
| (3,2722) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 32       | 0.22          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,2722) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 40       | 0.22          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 10       | 0.22          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 23       | 0.22          |
| (3,2697) | 1:23:A:GLU:HA  | 1:24:A:HIS:H   | 37       | 0.22          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 1        | 0.22          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 2        | 0.22          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 3        | 0.22          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 8        | 0.22          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 11       | 0.22          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 12       | 0.22          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 14       | 0.22          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 15       | 0.22          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 16       | 0.22          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 17       | 0.22          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 18       | 0.22          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 19       | 0.22          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 20       | 0.22          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 21       | 0.22          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 22       | 0.22          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 23       | 0.22          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 24       | 0.22          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 25       | 0.22          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 27       | 0.22          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 28       | 0.22          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 30       | 0.22          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 31       | 0.22          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 32       | 0.22          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 34       | 0.22          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 35       | 0.22          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 36       | 0.22          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 37       | 0.22          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 39       | 0.22          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 40       | 0.22          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 6        | 0.22          |
| (3,2602) | 1:36:A:ASP:HB2 | 1:37:A:ASP:H   | 1        | 0.22          |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 3        | 0.22          |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 9        | 0.22          |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 12       | 0.22          |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 14       | 0.22          |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 15       | 0.22          |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 21       | 0.22          |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 27       | 0.22          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,2554) | 1:92:A:ARG:HA  | 1:83:A:ALA:H   | 35       | 0.22          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 31       | 0.22          |
| (3,2538) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 4        | 0.22          |
| (3,2538) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 11       | 0.22          |
| (3,2538) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 14       | 0.22          |
| (3,2538) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 15       | 0.22          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 21       | 0.22          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 35       | 0.22          |
| (3,2485) | 1:9:A:PRO:HD3  | 1:9:A:PRO:HB3  | 22       | 0.22          |
| (3,2485) | 1:9:A:PRO:HD3  | 1:9:A:PRO:HB3  | 32       | 0.22          |
| (3,2485) | 1:9:A:PRO:HD3  | 1:9:A:PRO:HB3  | 35       | 0.22          |
| (3,2470) | 1:4:A:PRO:HB2  | 1:4:A:PRO:HD2  | 18       | 0.22          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 38       | 0.22          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 38       | 0.22          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 38       | 0.22          |
| (3,2326) | 1:80:A:SER:HB3 | 1:81:A:VAL:H   | 28       | 0.22          |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 5        | 0.22          |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 9        | 0.22          |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 22       | 0.22          |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 24       | 0.22          |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 27       | 0.22          |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 31       | 0.22          |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 40       | 0.22          |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 1        | 0.22          |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 7        | 0.22          |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 8        | 0.22          |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 15       | 0.22          |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 23       | 0.22          |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 37       | 0.22          |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 40       | 0.22          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1 | 4        | 0.22          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2 | 4        | 0.22          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1 | 6        | 0.22          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2 | 6        | 0.22          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1 | 15       | 0.22          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2 | 15       | 0.22          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1 | 16       | 0.22          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2 | 16       | 0.22          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1 | 31       | 0.22          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2 | 31       | 0.22          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1 | 39       | 0.22          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2 | 39       | 0.22          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (3,2239) | 1:18:A:ASN:HB3  | 1:18:A:ASN:H  | 1        | 0.22          |
| (3,2239) | 1:18:A:ASN:HB3  | 1:18:A:ASN:H  | 29       | 0.22          |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H  | 17       | 0.22          |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H  | 35       | 0.22          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 16       | 0.22          |
| (3,2154) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 33       | 0.22          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 1        | 0.22          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 1        | 0.22          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 1        | 0.22          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 2        | 0.22          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 2        | 0.22          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 2        | 0.22          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 3        | 0.22          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 3        | 0.22          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 3        | 0.22          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 4        | 0.22          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 4        | 0.22          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 4        | 0.22          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 6        | 0.22          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 6        | 0.22          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 6        | 0.22          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 7        | 0.22          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 7        | 0.22          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 7        | 0.22          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 10       | 0.22          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 10       | 0.22          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 10       | 0.22          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 11       | 0.22          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 11       | 0.22          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 11       | 0.22          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 12       | 0.22          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 12       | 0.22          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 12       | 0.22          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 13       | 0.22          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 13       | 0.22          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 13       | 0.22          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 14       | 0.22          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 14       | 0.22          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 14       | 0.22          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 15       | 0.22          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 15       | 0.22          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 15       | 0.22          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 17       | 0.22          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 17       | 0.22          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 17       | 0.22          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 19       | 0.22          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 19       | 0.22          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 19       | 0.22          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 21       | 0.22          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 21       | 0.22          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 21       | 0.22          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 22       | 0.22          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 22       | 0.22          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 22       | 0.22          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 23       | 0.22          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 23       | 0.22          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 23       | 0.22          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 24       | 0.22          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 24       | 0.22          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 24       | 0.22          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 25       | 0.22          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 25       | 0.22          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 25       | 0.22          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 26       | 0.22          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 26       | 0.22          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 26       | 0.22          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 29       | 0.22          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 29       | 0.22          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 29       | 0.22          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 30       | 0.22          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 30       | 0.22          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 30       | 0.22          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 33       | 0.22          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 33       | 0.22          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 33       | 0.22          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 34       | 0.22          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 34       | 0.22          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 34       | 0.22          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 35       | 0.22          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 35       | 0.22          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 35       | 0.22          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 36       | 0.22          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 36       | 0.22          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 36       | 0.22          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB  | 37       | 0.22          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB  | 37       | 0.22          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB  | 37       | 0.22          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB  | 39       | 0.22          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB  | 39       | 0.22          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB  | 39       | 0.22          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 18       | 0.22          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 18       | 0.22          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 18       | 0.22          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 37       | 0.22          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 37       | 0.22          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 37       | 0.22          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2 | 18       | 0.22          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2 | 18       | 0.22          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2 | 18       | 0.22          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 31       | 0.22          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 31       | 0.22          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 31       | 0.22          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 31       | 0.22          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 31       | 0.22          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 31       | 0.22          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 15       | 0.22          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 15       | 0.22          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 15       | 0.22          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 19       | 0.22          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 19       | 0.22          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 19       | 0.22          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 38       | 0.22          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 38       | 0.22          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 38       | 0.22          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 11       | 0.22          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 11       | 0.22          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 11       | 0.22          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 12       | 0.22          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 12       | 0.22          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 12       | 0.22          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 35       | 0.22          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 35       | 0.22          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 35       | 0.22          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 38       | 0.22          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 38       | 0.22          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 38       | 0.22          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA  | 5        | 0.22          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 9        | 0.22          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 9        | 0.22          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 9        | 0.22          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 13       | 0.22          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 13       | 0.22          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 13       | 0.22          |
| (3,1956) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 15       | 0.22          |
| (3,1956) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 15       | 0.22          |
| (3,1956) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 15       | 0.22          |
| (3,1938) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 2        | 0.22          |
| (3,1938) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 3        | 0.22          |
| (3,1938) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 8        | 0.22          |
| (3,1938) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 11       | 0.22          |
| (3,1938) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 12       | 0.22          |
| (3,1938) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 13       | 0.22          |
| (3,1938) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 14       | 0.22          |
| (3,1938) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 19       | 0.22          |
| (3,1938) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 21       | 0.22          |
| (3,1938) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 24       | 0.22          |
| (3,1938) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 28       | 0.22          |
| (3,1938) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 29       | 0.22          |
| (3,1938) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 33       | 0.22          |
| (3,1938) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 35       | 0.22          |
| (3,1938) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 38       | 0.22          |
| (3,1938) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 39       | 0.22          |
| (3,1938) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 40       | 0.22          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 2        | 0.22          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 4        | 0.22          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 15       | 0.22          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 23       | 0.22          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 34       | 0.22          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 35       | 0.22          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 40       | 0.22          |
| (3,1907) | 1:66:A:MET:HE1  | 1:43:A:TYR:H   | 4        | 0.22          |
| (3,1907) | 1:66:A:MET:HE2  | 1:43:A:TYR:H   | 4        | 0.22          |
| (3,1907) | 1:66:A:MET:HE3  | 1:43:A:TYR:H   | 4        | 0.22          |
| (3,1907) | 1:66:A:MET:HE1  | 1:43:A:TYR:H   | 21       | 0.22          |
| (3,1907) | 1:66:A:MET:HE2  | 1:43:A:TYR:H   | 21       | 0.22          |
| (3,1907) | 1:66:A:MET:HE3  | 1:43:A:TYR:H   | 21       | 0.22          |
| (3,1907) | 1:66:A:MET:HE1  | 1:43:A:TYR:H   | 28       | 0.22          |
| (3,1907) | 1:66:A:MET:HE2  | 1:43:A:TYR:H   | 28       | 0.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1907) | 1:66:A:MET:HE3  | 1:43:A:TYR:H    | 28       | 0.22          |
| (3,1907) | 1:66:A:MET:HE1  | 1:43:A:TYR:H    | 29       | 0.22          |
| (3,1907) | 1:66:A:MET:HE2  | 1:43:A:TYR:H    | 29       | 0.22          |
| (3,1907) | 1:66:A:MET:HE3  | 1:43:A:TYR:H    | 29       | 0.22          |
| (3,1828) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 11       | 0.22          |
| (3,1828) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 16       | 0.22          |
| (3,1828) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 17       | 0.22          |
| (3,1828) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 22       | 0.22          |
| (3,1828) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 31       | 0.22          |
| (3,1828) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 37       | 0.22          |
| (3,1815) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 11       | 0.22          |
| (3,1815) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 16       | 0.22          |
| (3,1815) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 17       | 0.22          |
| (3,1815) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 22       | 0.22          |
| (3,1815) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 31       | 0.22          |
| (3,1815) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 37       | 0.22          |
| (3,1781) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H    | 2        | 0.22          |
| (3,1781) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H    | 4        | 0.22          |
| (3,1781) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H    | 18       | 0.22          |
| (3,1721) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG11 | 24       | 0.22          |
| (3,1721) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG12 | 24       | 0.22          |
| (3,1721) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG13 | 24       | 0.22          |
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG11 | 24       | 0.22          |
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG12 | 24       | 0.22          |
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 24       | 0.22          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 24       | 0.22          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 24       | 0.22          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 24       | 0.22          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 1        | 0.22          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 1        | 0.22          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 1        | 0.22          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 4        | 0.22          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 4        | 0.22          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 4        | 0.22          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 5        | 0.22          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 5        | 0.22          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 5        | 0.22          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 8        | 0.22          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 8        | 0.22          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 8        | 0.22          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 15       | 0.22          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 15       | 0.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 15       | 0.22          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 28       | 0.22          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 28       | 0.22          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 28       | 0.22          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 28       | 0.22          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 28       | 0.22          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 28       | 0.22          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 28       | 0.22          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 28       | 0.22          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 28       | 0.22          |
| (3,1628) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2  | 25       | 0.22          |
| (3,1628) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2  | 25       | 0.22          |
| (3,1628) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2  | 25       | 0.22          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 6        | 0.22          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 6        | 0.22          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 6        | 0.22          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 12       | 0.22          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 12       | 0.22          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 12       | 0.22          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB   | 38       | 0.22          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB   | 38       | 0.22          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB   | 38       | 0.22          |
| (3,1540) | 1:39:A:ILE:HD11 | 1:40:A:VAL:H    | 2        | 0.22          |
| (3,1540) | 1:39:A:ILE:HD12 | 1:40:A:VAL:H    | 2        | 0.22          |
| (3,1540) | 1:39:A:ILE:HD13 | 1:40:A:VAL:H    | 2        | 0.22          |
| (3,1540) | 1:39:A:ILE:HD11 | 1:40:A:VAL:H    | 24       | 0.22          |
| (3,1540) | 1:39:A:ILE:HD12 | 1:40:A:VAL:H    | 24       | 0.22          |
| (3,1540) | 1:39:A:ILE:HD13 | 1:40:A:VAL:H    | 24       | 0.22          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1  | 1        | 0.22          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2  | 1        | 0.22          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1  | 1        | 0.22          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2  | 1        | 0.22          |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1  | 1        | 0.22          |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2  | 1        | 0.22          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1  | 5        | 0.22          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2  | 5        | 0.22          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1  | 5        | 0.22          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2  | 5        | 0.22          |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1  | 5        | 0.22          |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2  | 5        | 0.22          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 26       | 0.22          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H    | 36       | 0.22          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 8        | 0.22          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 8        | 0.22          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 8        | 0.22          |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 7        | 0.22          |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 7        | 0.22          |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 7        | 0.22          |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 9        | 0.22          |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 9        | 0.22          |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 9        | 0.22          |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 19       | 0.22          |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 19       | 0.22          |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 19       | 0.22          |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 22       | 0.22          |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 22       | 0.22          |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 22       | 0.22          |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 28       | 0.22          |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 28       | 0.22          |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 28       | 0.22          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 7        | 0.22          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 7        | 0.22          |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 7        | 0.22          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 8        | 0.22          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 8        | 0.22          |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 8        | 0.22          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H   | 21       | 0.22          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H   | 21       | 0.22          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H   | 21       | 0.22          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H   | 25       | 0.22          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H   | 25       | 0.22          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H   | 25       | 0.22          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H   | 28       | 0.22          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H   | 28       | 0.22          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H   | 28       | 0.22          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H   | 30       | 0.22          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H   | 30       | 0.22          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H   | 30       | 0.22          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H   | 32       | 0.22          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H   | 32       | 0.22          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H   | 32       | 0.22          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H   | 11       | 0.22          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H   | 11       | 0.22          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H   | 11       | 0.22          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H  | 16       | 0.22          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H  | 16       | 0.22          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H  | 16       | 0.22          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H  | 18       | 0.22          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H  | 18       | 0.22          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H  | 18       | 0.22          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H  | 20       | 0.22          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H  | 20       | 0.22          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H  | 20       | 0.22          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H  | 23       | 0.22          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H  | 23       | 0.22          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H  | 23       | 0.22          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H  | 27       | 0.22          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H  | 27       | 0.22          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H  | 27       | 0.22          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H  | 29       | 0.22          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H  | 29       | 0.22          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H  | 29       | 0.22          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H  | 33       | 0.22          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H  | 33       | 0.22          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H  | 33       | 0.22          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H  | 35       | 0.22          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H  | 35       | 0.22          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H  | 35       | 0.22          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H  | 40       | 0.22          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H  | 40       | 0.22          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H  | 40       | 0.22          |
| (3,1400) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA | 16       | 0.22          |
| (3,1400) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA | 16       | 0.22          |
| (3,1400) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA | 16       | 0.22          |
| (3,1400) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA | 29       | 0.22          |
| (3,1400) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA | 29       | 0.22          |
| (3,1400) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA | 29       | 0.22          |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H  | 5        | 0.22          |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H  | 5        | 0.22          |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H  | 5        | 0.22          |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H  | 8        | 0.22          |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H  | 8        | 0.22          |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H  | 8        | 0.22          |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H  | 18       | 0.22          |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H  | 18       | 0.22          |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H  | 18       | 0.22          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 26       | 0.22          |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 26       | 0.22          |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 26       | 0.22          |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 31       | 0.22          |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 31       | 0.22          |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 31       | 0.22          |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 37       | 0.22          |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 37       | 0.22          |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 37       | 0.22          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 23       | 0.22          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 23       | 0.22          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 23       | 0.22          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 26       | 0.22          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 26       | 0.22          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 26       | 0.22          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 35       | 0.22          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 35       | 0.22          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 35       | 0.22          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 40       | 0.22          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 40       | 0.22          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 40       | 0.22          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 2        | 0.22          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 3        | 0.22          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 4        | 0.22          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 5        | 0.22          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 6        | 0.22          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 7        | 0.22          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 8        | 0.22          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 10       | 0.22          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 11       | 0.22          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 12       | 0.22          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 14       | 0.22          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 15       | 0.22          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 17       | 0.22          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 18       | 0.22          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 19       | 0.22          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 23       | 0.22          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 24       | 0.22          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 25       | 0.22          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 27       | 0.22          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 28       | 0.22          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 29       | 0.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 31       | 0.22          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 32       | 0.22          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 33       | 0.22          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 34       | 0.22          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 36       | 0.22          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 37       | 0.22          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 39       | 0.22          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 40       | 0.22          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 11       | 0.22          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 11       | 0.22          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 11       | 0.22          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 16       | 0.22          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 16       | 0.22          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 16       | 0.22          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 11       | 0.22          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 11       | 0.22          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 11       | 0.22          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 16       | 0.22          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 16       | 0.22          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 16       | 0.22          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 16       | 0.22          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 16       | 0.22          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 16       | 0.22          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 40       | 0.22          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 40       | 0.22          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 40       | 0.22          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 2        | 0.22          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 2        | 0.22          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 2        | 0.22          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 9        | 0.22          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 9        | 0.22          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 9        | 0.22          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 10       | 0.22          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 10       | 0.22          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 10       | 0.22          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 14       | 0.22          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 14       | 0.22          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 14       | 0.22          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 15       | 0.22          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 15       | 0.22          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 15       | 0.22          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 35       | 0.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 35       | 0.22          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 35       | 0.22          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 37       | 0.22          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 37       | 0.22          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 37       | 0.22          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 10       | 0.22          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 14       | 0.22          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 16       | 0.22          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 19       | 0.22          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 23       | 0.22          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 24       | 0.22          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 40       | 0.22          |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 1        | 0.22          |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 25       | 0.22          |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 35       | 0.22          |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 36       | 0.22          |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 39       | 0.22          |
| (3,1188) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 13       | 0.22          |
| (3,1188) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 34       | 0.22          |
| (3,1173) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 2        | 0.22          |
| (3,1173) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 4        | 0.22          |
| (3,1173) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 10       | 0.22          |
| (3,1173) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 13       | 0.22          |
| (3,1173) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 16       | 0.22          |
| (3,1173) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 24       | 0.22          |
| (3,1173) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 29       | 0.22          |
| (3,1173) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 35       | 0.22          |
| (3,1173) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 40       | 0.22          |
| (3,1167) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 1        | 0.22          |
| (3,1167) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 2        | 0.22          |
| (3,1167) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 3        | 0.22          |
| (3,1167) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 4        | 0.22          |
| (3,1167) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 8        | 0.22          |
| (3,1167) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 10       | 0.22          |
| (3,1167) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 16       | 0.22          |
| (3,1167) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 20       | 0.22          |
| (3,1167) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 26       | 0.22          |
| (3,1166) | 1:97:A:LEU:H    | 1:29:A:PHE:HE1  | 4        | 0.22          |
| (3,1166) | 1:97:A:LEU:H    | 1:29:A:PHE:HE2  | 4        | 0.22          |
| (3,1166) | 1:97:A:LEU:H    | 1:29:A:PHE:HE1  | 8        | 0.22          |
| (3,1166) | 1:97:A:LEU:H    | 1:29:A:PHE:HE2  | 8        | 0.22          |
| (3,970)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 1        | 0.22          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,970) | 1:21:A:VAL:H | 1:20:A:VAL:HB   | 2        | 0.22          |
| (3,970) | 1:21:A:VAL:H | 1:20:A:VAL:HB   | 8        | 0.22          |
| (3,970) | 1:21:A:VAL:H | 1:20:A:VAL:HB   | 13       | 0.22          |
| (3,970) | 1:21:A:VAL:H | 1:20:A:VAL:HB   | 14       | 0.22          |
| (3,970) | 1:21:A:VAL:H | 1:20:A:VAL:HB   | 15       | 0.22          |
| (3,970) | 1:21:A:VAL:H | 1:20:A:VAL:HB   | 17       | 0.22          |
| (3,970) | 1:21:A:VAL:H | 1:20:A:VAL:HB   | 18       | 0.22          |
| (3,970) | 1:21:A:VAL:H | 1:20:A:VAL:HB   | 19       | 0.22          |
| (3,970) | 1:21:A:VAL:H | 1:20:A:VAL:HB   | 22       | 0.22          |
| (3,970) | 1:21:A:VAL:H | 1:20:A:VAL:HB   | 26       | 0.22          |
| (3,970) | 1:21:A:VAL:H | 1:20:A:VAL:HB   | 27       | 0.22          |
| (3,970) | 1:21:A:VAL:H | 1:20:A:VAL:HB   | 28       | 0.22          |
| (3,970) | 1:21:A:VAL:H | 1:20:A:VAL:HB   | 29       | 0.22          |
| (3,970) | 1:21:A:VAL:H | 1:20:A:VAL:HB   | 32       | 0.22          |
| (3,970) | 1:21:A:VAL:H | 1:20:A:VAL:HB   | 33       | 0.22          |
| (3,970) | 1:21:A:VAL:H | 1:20:A:VAL:HB   | 36       | 0.22          |
| (3,970) | 1:21:A:VAL:H | 1:20:A:VAL:HB   | 38       | 0.22          |
| (3,970) | 1:21:A:VAL:H | 1:20:A:VAL:HB   | 39       | 0.22          |
| (3,970) | 1:21:A:VAL:H | 1:20:A:VAL:HB   | 40       | 0.22          |
| (3,933) | 1:98:A:LYS:H | 1:19:A:ILE:HB   | 8        | 0.22          |
| (3,933) | 1:98:A:LYS:H | 1:19:A:ILE:HB   | 21       | 0.22          |
| (3,933) | 1:98:A:LYS:H | 1:19:A:ILE:HB   | 39       | 0.22          |
| (3,920) | 1:37:A:ASP:H | 1:36:A:ASP:HB2  | 1        | 0.22          |
| (3,919) | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 3        | 0.22          |
| (3,919) | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 9        | 0.22          |
| (3,919) | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 12       | 0.22          |
| (3,919) | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 14       | 0.22          |
| (3,919) | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 15       | 0.22          |
| (3,919) | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 21       | 0.22          |
| (3,919) | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 27       | 0.22          |
| (3,889) | 1:80:A:SER:H | 1:43:A:TYR:HB3  | 20       | 0.22          |
| (3,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2   | 7        | 0.22          |
| (3,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2   | 8        | 0.22          |
| (3,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 5        | 0.22          |
| (3,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 40       | 0.22          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 33       | 0.22          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 33       | 0.22          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 33       | 0.22          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 36       | 0.22          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 36       | 0.22          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 36       | 0.22          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 11       | 0.22          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG22 | 11       | 0.22          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG23 | 11       | 0.22          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG21 | 22       | 0.22          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG22 | 22       | 0.22          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG23 | 22       | 0.22          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG21 | 23       | 0.22          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG22 | 23       | 0.22          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG23 | 23       | 0.22          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG21 | 28       | 0.22          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG22 | 28       | 0.22          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG23 | 28       | 0.22          |
| (3,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 12       | 0.22          |
| (3,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 14       | 0.22          |
| (3,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 19       | 0.22          |
| (3,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 21       | 0.22          |
| (3,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 29       | 0.22          |
| (3,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 33       | 0.22          |
| (3,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 40       | 0.22          |
| (3,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3  | 10       | 0.22          |
| (3,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3  | 15       | 0.22          |
| (3,685) | 1:23:A:GLU:H  | 1:23:A:GLU:HG3  | 28       | 0.22          |
| (3,685) | 1:23:A:GLU:H  | 1:23:A:GLU:HG3  | 37       | 0.22          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 1        | 0.22          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 3        | 0.22          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 8        | 0.22          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 12       | 0.22          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 13       | 0.22          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 18       | 0.22          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 20       | 0.22          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 23       | 0.22          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 25       | 0.22          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 30       | 0.22          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 38       | 0.22          |
| (3,590) | 1:3:A:ASP:H   | 1:2:A:ILE:HA    | 2        | 0.22          |
| (3,590) | 1:3:A:ASP:H   | 1:2:A:ILE:HA    | 5        | 0.22          |
| (3,589) | 1:93:A:SER:H  | 1:92:A:ARG:HG2  | 14       | 0.22          |
| (3,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 10       | 0.22          |
| (3,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2  | 10       | 0.22          |
| (3,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 17       | 0.22          |
| (3,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2  | 17       | 0.22          |
| (3,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 27       | 0.22          |
| (3,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2  | 27       | 0.22          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1  | 38       | 0.22          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2  | 38       | 0.22          |
| (3,556) | 1:47:A:THR:H | 1:48:A:GLU:H    | 4        | 0.22          |
| (3,556) | 1:47:A:THR:H | 1:48:A:GLU:H    | 5        | 0.22          |
| (3,556) | 1:47:A:THR:H | 1:48:A:GLU:H    | 11       | 0.22          |
| (3,556) | 1:47:A:THR:H | 1:48:A:GLU:H    | 16       | 0.22          |
| (3,556) | 1:47:A:THR:H | 1:48:A:GLU:H    | 31       | 0.22          |
| (3,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 31       | 0.22          |
| (3,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 2        | 0.22          |
| (3,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 4        | 0.22          |
| (3,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 11       | 0.22          |
| (3,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 12       | 0.22          |
| (3,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 30       | 0.22          |
| (3,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 32       | 0.22          |
| (3,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 35       | 0.22          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 15       | 0.22          |
| (3,513) | 1:67:A:THR:H | 1:66:A:MET:HG3  | 2        | 0.22          |
| (3,513) | 1:67:A:THR:H | 1:66:A:MET:HG3  | 40       | 0.22          |
| (3,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2  | 4        | 0.22          |
| (3,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2  | 8        | 0.22          |
| (3,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2  | 11       | 0.22          |
| (3,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2  | 12       | 0.22          |
| (3,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2  | 31       | 0.22          |
| (3,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2  | 32       | 0.22          |
| (3,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2  | 33       | 0.22          |
| (3,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2  | 38       | 0.22          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 20       | 0.22          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 23       | 0.22          |
| (3,366) | 1:18:A:ASN:H | 1:18:A:ASN:HB3  | 1        | 0.22          |
| (3,366) | 1:18:A:ASN:H | 1:18:A:ASN:HB3  | 29       | 0.22          |
| (3,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 22       | 0.22          |
| (3,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 23       | 0.22          |
| (3,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 40       | 0.22          |
| (3,248) | 1:95:A:ALA:H | 1:94:A:THR:HB   | 28       | 0.22          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 5        | 0.22          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 5        | 0.22          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 16       | 0.22          |
| (3,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 16       | 0.22          |
| (3,135) | 1:39:A:ILE:H | 1:39:A:ILE:HG13 | 4        | 0.22          |
| (3,135) | 1:39:A:ILE:H | 1:39:A:ILE:HG13 | 5        | 0.22          |
| (3,135) | 1:39:A:ILE:H | 1:39:A:ILE:HG13 | 13       | 0.22          |
| (3,135) | 1:39:A:ILE:H | 1:39:A:ILE:HG13 | 17       | 0.22          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,131)  | 1:39:A:ILE:H   | 1:39:A:ILE:HA   | 7        | 0.22          |
| (3,131)  | 1:39:A:ILE:H   | 1:39:A:ILE:HA   | 13       | 0.22          |
| (3,131)  | 1:39:A:ILE:H   | 1:39:A:ILE:HA   | 16       | 0.22          |
| (3,131)  | 1:39:A:ILE:H   | 1:39:A:ILE:HA   | 19       | 0.22          |
| (3,131)  | 1:39:A:ILE:H   | 1:39:A:ILE:HA   | 21       | 0.22          |
| (3,131)  | 1:39:A:ILE:H   | 1:39:A:ILE:HA   | 28       | 0.22          |
| (3,131)  | 1:39:A:ILE:H   | 1:39:A:ILE:HA   | 38       | 0.22          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 8        | 0.22          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 8        | 0.22          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 8        | 0.22          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 11       | 0.22          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 11       | 0.22          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 11       | 0.22          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 12       | 0.22          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 12       | 0.22          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 12       | 0.22          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 24       | 0.22          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 24       | 0.22          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 24       | 0.22          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 27       | 0.22          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 27       | 0.22          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 27       | 0.22          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 30       | 0.22          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 30       | 0.22          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 30       | 0.22          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 34       | 0.22          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 34       | 0.22          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 34       | 0.22          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 39       | 0.22          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 39       | 0.22          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 39       | 0.22          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 13       | 0.22          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 13       | 0.22          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 15       | 0.22          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 15       | 0.22          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 25       | 0.22          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 25       | 0.22          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 29       | 0.22          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 29       | 0.22          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 36       | 0.22          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 36       | 0.22          |
| (1,3211) | 1:69:A:HIS:HE1 | 1:67:A:THR:HB   | 17       | 0.22          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 7        | 0.22          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 7        | 0.22          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 17       | 0.22          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 18       | 0.22          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 20       | 0.22          |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2  | 34       | 0.22          |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2  | 34       | 0.22          |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 4        | 0.22          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 4        | 0.22          |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 17       | 0.22          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 17       | 0.22          |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 20       | 0.22          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 20       | 0.22          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 34       | 0.22          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 34       | 0.22          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 34       | 0.22          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 34       | 0.22          |
| (1,3048) | 1:60:A:ASP:HB2 | 1:63:A:CYS:HB2  | 37       | 0.22          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 24       | 0.22          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 13       | 0.22          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 13       | 0.22          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 13       | 0.22          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 34       | 0.22          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 34       | 0.22          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 34       | 0.22          |
| (1,2996) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 1        | 0.22          |
| (1,2968) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3  | 1        | 0.22          |
| (1,2968) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3  | 3        | 0.22          |
| (1,2968) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3  | 4        | 0.22          |
| (1,2968) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3  | 5        | 0.22          |
| (1,2968) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3  | 6        | 0.22          |
| (1,2968) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3  | 7        | 0.22          |
| (1,2968) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3  | 10       | 0.22          |
| (1,2968) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3  | 11       | 0.22          |
| (1,2968) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3  | 12       | 0.22          |
| (1,2968) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3  | 13       | 0.22          |
| (1,2968) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3  | 14       | 0.22          |
| (1,2968) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3  | 15       | 0.22          |
| (1,2968) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3  | 18       | 0.22          |
| (1,2968) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3  | 23       | 0.22          |
| (1,2968) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3  | 25       | 0.22          |
| (1,2968) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD3  | 26       | 0.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2968) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 27       | 0.22          |
| (1,2968) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 29       | 0.22          |
| (1,2968) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 30       | 0.22          |
| (1,2968) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 31       | 0.22          |
| (1,2968) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 32       | 0.22          |
| (1,2968) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 33       | 0.22          |
| (1,2968) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 34       | 0.22          |
| (1,2968) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 36       | 0.22          |
| (1,2968) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 37       | 0.22          |
| (1,2968) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 38       | 0.22          |
| (1,2961) | 1:44:A:LYS:HE2  | 1:44:A:LYS:HG2  | 2        | 0.22          |
| (1,2961) | 1:44:A:LYS:HE2  | 1:44:A:LYS:HG2  | 20       | 0.22          |
| (1,2918) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 3        | 0.22          |
| (1,2918) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 16       | 0.22          |
| (1,2857) | 1:92:A:ARG:HB3  | 1:92:A:ARG:HG3  | 1        | 0.22          |
| (1,2857) | 1:92:A:ARG:HB3  | 1:92:A:ARG:HG3  | 9        | 0.22          |
| (1,2857) | 1:92:A:ARG:HB3  | 1:92:A:ARG:HG3  | 10       | 0.22          |
| (1,2857) | 1:92:A:ARG:HB3  | 1:92:A:ARG:HG3  | 13       | 0.22          |
| (1,2857) | 1:92:A:ARG:HB3  | 1:92:A:ARG:HG3  | 14       | 0.22          |
| (1,2857) | 1:92:A:ARG:HB3  | 1:92:A:ARG:HG3  | 18       | 0.22          |
| (1,2857) | 1:92:A:ARG:HB3  | 1:92:A:ARG:HG3  | 35       | 0.22          |
| (1,2857) | 1:92:A:ARG:HB3  | 1:92:A:ARG:HG3  | 38       | 0.22          |
| (1,2802) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HB2  | 28       | 0.22          |
| (1,2801) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HG2  | 2        | 0.22          |
| (1,2801) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HG2  | 5        | 0.22          |
| (1,2801) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HG2  | 8        | 0.22          |
| (1,2801) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HG2  | 9        | 0.22          |
| (1,2801) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HG2  | 16       | 0.22          |
| (1,2801) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HG2  | 25       | 0.22          |
| (1,2801) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HG2  | 30       | 0.22          |
| (1,2801) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HG2  | 33       | 0.22          |
| (1,2801) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HG2  | 37       | 0.22          |
| (1,2796) | 1:15:A:ARG:HG3  | 1:15:A:ARG:HB3  | 2        | 0.22          |
| (1,2796) | 1:15:A:ARG:HG3  | 1:15:A:ARG:HB3  | 5        | 0.22          |
| (1,2796) | 1:15:A:ARG:HG3  | 1:15:A:ARG:HB3  | 8        | 0.22          |
| (1,2796) | 1:15:A:ARG:HG3  | 1:15:A:ARG:HB3  | 11       | 0.22          |
| (1,2796) | 1:15:A:ARG:HG3  | 1:15:A:ARG:HB3  | 30       | 0.22          |
| (1,2796) | 1:15:A:ARG:HG3  | 1:15:A:ARG:HB3  | 31       | 0.22          |
| (1,2796) | 1:15:A:ARG:HG3  | 1:15:A:ARG:HB3  | 33       | 0.22          |
| (1,2796) | 1:15:A:ARG:HG3  | 1:15:A:ARG:HB3  | 38       | 0.22          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 12       | 0.22          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 13       | 0.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 17       | 0.22          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 19       | 0.22          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 20       | 0.22          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 22       | 0.22          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 24       | 0.22          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 28       | 0.22          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 30       | 0.22          |
| (1,2780) | 1:100:A:GLU:HG2 | 1:100:A:GLU:HG3 | 34       | 0.22          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 12       | 0.22          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 13       | 0.22          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 17       | 0.22          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 19       | 0.22          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 20       | 0.22          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 22       | 0.22          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 24       | 0.22          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 28       | 0.22          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 30       | 0.22          |
| (1,2779) | 1:100:A:GLU:HG3 | 1:100:A:GLU:HG2 | 34       | 0.22          |
| (1,2754) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 24       | 0.22          |
| (1,2754) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 25       | 0.22          |
| (1,2718) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 4        | 0.22          |
| (1,2718) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 7        | 0.22          |
| (1,2718) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 17       | 0.22          |
| (1,2718) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 23       | 0.22          |
| (1,2718) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 28       | 0.22          |
| (1,2718) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 32       | 0.22          |
| (1,2718) | 1:48:A:GLU:HG2  | 1:48:A:GLU:HA   | 40       | 0.22          |
| (1,2693) | 1:23:A:GLU:HA   | 1:24:A:HIS:H    | 10       | 0.22          |
| (1,2693) | 1:23:A:GLU:HA   | 1:24:A:HIS:H    | 23       | 0.22          |
| (1,2693) | 1:23:A:GLU:HA   | 1:24:A:HIS:H    | 37       | 0.22          |
| (1,2668) | 1:25:A:GLN:HG3  | 1:25:A:GLN:HA   | 1        | 0.22          |
| (1,2668) | 1:25:A:GLN:HG3  | 1:25:A:GLN:HA   | 2        | 0.22          |
| (1,2668) | 1:25:A:GLN:HG3  | 1:25:A:GLN:HA   | 3        | 0.22          |
| (1,2668) | 1:25:A:GLN:HG3  | 1:25:A:GLN:HA   | 8        | 0.22          |
| (1,2668) | 1:25:A:GLN:HG3  | 1:25:A:GLN:HA   | 11       | 0.22          |
| (1,2668) | 1:25:A:GLN:HG3  | 1:25:A:GLN:HA   | 12       | 0.22          |
| (1,2668) | 1:25:A:GLN:HG3  | 1:25:A:GLN:HA   | 14       | 0.22          |
| (1,2668) | 1:25:A:GLN:HG3  | 1:25:A:GLN:HA   | 15       | 0.22          |
| (1,2668) | 1:25:A:GLN:HG3  | 1:25:A:GLN:HA   | 16       | 0.22          |
| (1,2668) | 1:25:A:GLN:HG3  | 1:25:A:GLN:HA   | 17       | 0.22          |
| (1,2668) | 1:25:A:GLN:HG3  | 1:25:A:GLN:HA   | 18       | 0.22          |
| (1,2668) | 1:25:A:GLN:HG3  | 1:25:A:GLN:HA   | 19       | 0.22          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,2668) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 20       | 0.22          |
| (1,2668) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 21       | 0.22          |
| (1,2668) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 22       | 0.22          |
| (1,2668) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 23       | 0.22          |
| (1,2668) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 24       | 0.22          |
| (1,2668) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 25       | 0.22          |
| (1,2668) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 27       | 0.22          |
| (1,2668) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 28       | 0.22          |
| (1,2668) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 30       | 0.22          |
| (1,2668) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 31       | 0.22          |
| (1,2668) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 32       | 0.22          |
| (1,2668) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 34       | 0.22          |
| (1,2668) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 35       | 0.22          |
| (1,2668) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 36       | 0.22          |
| (1,2668) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 37       | 0.22          |
| (1,2668) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 39       | 0.22          |
| (1,2668) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 40       | 0.22          |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 6        | 0.22          |
| (1,2598) | 1:36:A:ASP:HB2 | 1:37:A:ASP:H   | 1        | 0.22          |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 3        | 0.22          |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 9        | 0.22          |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 12       | 0.22          |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 14       | 0.22          |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 15       | 0.22          |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 21       | 0.22          |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 27       | 0.22          |
| (1,2550) | 1:92:A:ARG:HA  | 1:83:A:ALA:H   | 35       | 0.22          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 31       | 0.22          |
| (1,2534) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 4        | 0.22          |
| (1,2534) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 11       | 0.22          |
| (1,2534) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 14       | 0.22          |
| (1,2534) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 15       | 0.22          |
| (1,2485) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 21       | 0.22          |
| (1,2485) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 35       | 0.22          |
| (1,2467) | 1:4:A:PRO:HB2  | 1:4:A:PRO:HD2  | 18       | 0.22          |
| (1,2402) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 38       | 0.22          |
| (1,2402) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 38       | 0.22          |
| (1,2402) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 38       | 0.22          |
| (1,2323) | 1:80:A:SER:HB3 | 1:81:A:VAL:H   | 28       | 0.22          |
| (1,2322) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 5        | 0.22          |
| (1,2322) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 9        | 0.22          |
| (1,2322) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 22       | 0.22          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2322) | 1:80:A:SER:HB2  | 1:81:A:VAL:H   | 24       | 0.22          |
| (1,2322) | 1:80:A:SER:HB2  | 1:81:A:VAL:H   | 27       | 0.22          |
| (1,2322) | 1:80:A:SER:HB2  | 1:81:A:VAL:H   | 31       | 0.22          |
| (1,2322) | 1:80:A:SER:HB2  | 1:81:A:VAL:H   | 40       | 0.22          |
| (1,2286) | 1:96:A:GLU:HG2  | 1:97:A:LEU:H   | 1        | 0.22          |
| (1,2286) | 1:96:A:GLU:HG2  | 1:97:A:LEU:H   | 7        | 0.22          |
| (1,2286) | 1:96:A:GLU:HG2  | 1:97:A:LEU:H   | 8        | 0.22          |
| (1,2286) | 1:96:A:GLU:HG2  | 1:97:A:LEU:H   | 15       | 0.22          |
| (1,2286) | 1:96:A:GLU:HG2  | 1:97:A:LEU:H   | 23       | 0.22          |
| (1,2286) | 1:96:A:GLU:HG2  | 1:97:A:LEU:H   | 37       | 0.22          |
| (1,2286) | 1:96:A:GLU:HG2  | 1:97:A:LEU:H   | 40       | 0.22          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1 | 4        | 0.22          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2 | 4        | 0.22          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1 | 6        | 0.22          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2 | 6        | 0.22          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1 | 15       | 0.22          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2 | 15       | 0.22          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1 | 16       | 0.22          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2 | 16       | 0.22          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1 | 31       | 0.22          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2 | 31       | 0.22          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1 | 39       | 0.22          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2 | 39       | 0.22          |
| (1,2236) | 1:18:A:ASN:HB3  | 1:18:A:ASN:H   | 1        | 0.22          |
| (1,2236) | 1:18:A:ASN:HB3  | 1:18:A:ASN:H   | 29       | 0.22          |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H   | 17       | 0.22          |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H   | 35       | 0.22          |
| (1,2151) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3  | 16       | 0.22          |
| (1,2151) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3  | 33       | 0.22          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB  | 1        | 0.22          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB  | 1        | 0.22          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB  | 1        | 0.22          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB  | 2        | 0.22          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB  | 2        | 0.22          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB  | 2        | 0.22          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB  | 3        | 0.22          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB  | 3        | 0.22          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB  | 3        | 0.22          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB  | 4        | 0.22          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB  | 4        | 0.22          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB  | 4        | 0.22          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB  | 6        | 0.22          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 6        | 0.22          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 6        | 0.22          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 7        | 0.22          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 7        | 0.22          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 7        | 0.22          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 10       | 0.22          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 10       | 0.22          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 10       | 0.22          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 11       | 0.22          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 11       | 0.22          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 11       | 0.22          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 12       | 0.22          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 12       | 0.22          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 12       | 0.22          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 13       | 0.22          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 13       | 0.22          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 13       | 0.22          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 14       | 0.22          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 14       | 0.22          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 14       | 0.22          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 15       | 0.22          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 15       | 0.22          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 15       | 0.22          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 17       | 0.22          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 17       | 0.22          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 17       | 0.22          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 19       | 0.22          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 19       | 0.22          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 19       | 0.22          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 21       | 0.22          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 21       | 0.22          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 21       | 0.22          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 22       | 0.22          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 22       | 0.22          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 22       | 0.22          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 23       | 0.22          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 23       | 0.22          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 23       | 0.22          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 24       | 0.22          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB | 24       | 0.22          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB | 24       | 0.22          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB | 25       | 0.22          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB  | 25       | 0.22          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB  | 25       | 0.22          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB  | 26       | 0.22          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB  | 26       | 0.22          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB  | 26       | 0.22          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB  | 29       | 0.22          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB  | 29       | 0.22          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB  | 29       | 0.22          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB  | 30       | 0.22          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB  | 30       | 0.22          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB  | 30       | 0.22          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB  | 33       | 0.22          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB  | 33       | 0.22          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB  | 33       | 0.22          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB  | 34       | 0.22          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB  | 34       | 0.22          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB  | 34       | 0.22          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB  | 35       | 0.22          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB  | 35       | 0.22          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB  | 35       | 0.22          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB  | 36       | 0.22          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB  | 36       | 0.22          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB  | 36       | 0.22          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB  | 37       | 0.22          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB  | 37       | 0.22          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB  | 37       | 0.22          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB  | 39       | 0.22          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB  | 39       | 0.22          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB  | 39       | 0.22          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 18       | 0.22          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 18       | 0.22          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 18       | 0.22          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 37       | 0.22          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 37       | 0.22          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 37       | 0.22          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2 | 18       | 0.22          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2 | 18       | 0.22          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2 | 18       | 0.22          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 31       | 0.22          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 31       | 0.22          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 31       | 0.22          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 31       | 0.22          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 31       | 0.22          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 31       | 0.22          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 15       | 0.22          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 15       | 0.22          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 15       | 0.22          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 19       | 0.22          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 19       | 0.22          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 19       | 0.22          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 38       | 0.22          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 38       | 0.22          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 38       | 0.22          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 11       | 0.22          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 11       | 0.22          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 11       | 0.22          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 12       | 0.22          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 12       | 0.22          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 12       | 0.22          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 35       | 0.22          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 35       | 0.22          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 35       | 0.22          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 38       | 0.22          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 38       | 0.22          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 38       | 0.22          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA  | 5        | 0.22          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 9        | 0.22          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 9        | 0.22          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 9        | 0.22          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 13       | 0.22          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 13       | 0.22          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 13       | 0.22          |
| (1,1953) | 1:68:A:ILE:HD11 | 1:68:A:ILE:HA  | 15       | 0.22          |
| (1,1953) | 1:68:A:ILE:HD12 | 1:68:A:ILE:HA  | 15       | 0.22          |
| (1,1953) | 1:68:A:ILE:HD13 | 1:68:A:ILE:HA  | 15       | 0.22          |
| (1,1935) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 2        | 0.22          |
| (1,1935) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 3        | 0.22          |
| (1,1935) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 8        | 0.22          |
| (1,1935) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 11       | 0.22          |
| (1,1935) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 12       | 0.22          |
| (1,1935) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 13       | 0.22          |
| (1,1935) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 14       | 0.22          |
| (1,1935) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 19       | 0.22          |
| (1,1935) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 21       | 0.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1935) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2  | 24       | 0.22          |
| (1,1935) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2  | 28       | 0.22          |
| (1,1935) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2  | 29       | 0.22          |
| (1,1935) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2  | 33       | 0.22          |
| (1,1935) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2  | 35       | 0.22          |
| (1,1935) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2  | 38       | 0.22          |
| (1,1935) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2  | 39       | 0.22          |
| (1,1935) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2  | 40       | 0.22          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2  | 2        | 0.22          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2  | 4        | 0.22          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2  | 15       | 0.22          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2  | 23       | 0.22          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2  | 34       | 0.22          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2  | 35       | 0.22          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2  | 40       | 0.22          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 12       | 0.22          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 12       | 0.22          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 12       | 0.22          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 12       | 0.22          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 12       | 0.22          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 12       | 0.22          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 12       | 0.22          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 12       | 0.22          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 12       | 0.22          |
| (1,1904) | 1:66:A:MET:HE1  | 1:43:A:TYR:H    | 4        | 0.22          |
| (1,1904) | 1:66:A:MET:HE2  | 1:43:A:TYR:H    | 4        | 0.22          |
| (1,1904) | 1:66:A:MET:HE3  | 1:43:A:TYR:H    | 4        | 0.22          |
| (1,1904) | 1:66:A:MET:HE1  | 1:43:A:TYR:H    | 21       | 0.22          |
| (1,1904) | 1:66:A:MET:HE2  | 1:43:A:TYR:H    | 21       | 0.22          |
| (1,1904) | 1:66:A:MET:HE3  | 1:43:A:TYR:H    | 21       | 0.22          |
| (1,1904) | 1:66:A:MET:HE1  | 1:43:A:TYR:H    | 28       | 0.22          |
| (1,1904) | 1:66:A:MET:HE2  | 1:43:A:TYR:H    | 28       | 0.22          |
| (1,1904) | 1:66:A:MET:HE3  | 1:43:A:TYR:H    | 28       | 0.22          |
| (1,1904) | 1:66:A:MET:HE1  | 1:43:A:TYR:H    | 29       | 0.22          |
| (1,1904) | 1:66:A:MET:HE2  | 1:43:A:TYR:H    | 29       | 0.22          |
| (1,1904) | 1:66:A:MET:HE3  | 1:43:A:TYR:H    | 29       | 0.22          |
| (1,1825) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 11       | 0.22          |
| (1,1825) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 16       | 0.22          |
| (1,1825) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 17       | 0.22          |
| (1,1825) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 22       | 0.22          |
| (1,1825) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 31       | 0.22          |
| (1,1825) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 37       | 0.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1812) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 11       | 0.22          |
| (1,1812) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 16       | 0.22          |
| (1,1812) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 17       | 0.22          |
| (1,1812) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 22       | 0.22          |
| (1,1812) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 31       | 0.22          |
| (1,1812) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 37       | 0.22          |
| (1,1778) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H    | 2        | 0.22          |
| (1,1778) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H    | 4        | 0.22          |
| (1,1778) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H    | 18       | 0.22          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG11 | 24       | 0.22          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG12 | 24       | 0.22          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG13 | 24       | 0.22          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG11 | 24       | 0.22          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG12 | 24       | 0.22          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 24       | 0.22          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 24       | 0.22          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 24       | 0.22          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 24       | 0.22          |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 1        | 0.22          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 1        | 0.22          |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 1        | 0.22          |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 4        | 0.22          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 4        | 0.22          |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 4        | 0.22          |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 5        | 0.22          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 5        | 0.22          |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 5        | 0.22          |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 8        | 0.22          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 8        | 0.22          |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 8        | 0.22          |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 15       | 0.22          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 15       | 0.22          |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 15       | 0.22          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 28       | 0.22          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 28       | 0.22          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 28       | 0.22          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 28       | 0.22          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 28       | 0.22          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 28       | 0.22          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 28       | 0.22          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 28       | 0.22          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 28       | 0.22          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1624) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2 | 25       | 0.22          |
| (1,1624) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2 | 25       | 0.22          |
| (1,1624) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2 | 25       | 0.22          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2 | 6        | 0.22          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 6        | 0.22          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 6        | 0.22          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2 | 12       | 0.22          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 12       | 0.22          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 12       | 0.22          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB  | 38       | 0.22          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB  | 38       | 0.22          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB  | 38       | 0.22          |
| (1,1536) | 1:39:A:ILE:HD11 | 1:40:A:VAL:H   | 2        | 0.22          |
| (1,1536) | 1:39:A:ILE:HD12 | 1:40:A:VAL:H   | 2        | 0.22          |
| (1,1536) | 1:39:A:ILE:HD13 | 1:40:A:VAL:H   | 2        | 0.22          |
| (1,1536) | 1:39:A:ILE:HD11 | 1:40:A:VAL:H   | 24       | 0.22          |
| (1,1536) | 1:39:A:ILE:HD12 | 1:40:A:VAL:H   | 24       | 0.22          |
| (1,1536) | 1:39:A:ILE:HD13 | 1:40:A:VAL:H   | 24       | 0.22          |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1 | 1        | 0.22          |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2 | 1        | 0.22          |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1 | 1        | 0.22          |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2 | 1        | 0.22          |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1 | 1        | 0.22          |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2 | 1        | 0.22          |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1 | 5        | 0.22          |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2 | 5        | 0.22          |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1 | 5        | 0.22          |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2 | 5        | 0.22          |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1 | 5        | 0.22          |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2 | 5        | 0.22          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 26       | 0.22          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 36       | 0.22          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 8        | 0.22          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 8        | 0.22          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 8        | 0.22          |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 7        | 0.22          |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 7        | 0.22          |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 7        | 0.22          |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 9        | 0.22          |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 9        | 0.22          |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 9        | 0.22          |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 19       | 0.22          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 19       | 0.22          |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 19       | 0.22          |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 22       | 0.22          |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 22       | 0.22          |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 22       | 0.22          |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 28       | 0.22          |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 28       | 0.22          |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 28       | 0.22          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 7        | 0.22          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 7        | 0.22          |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 7        | 0.22          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 8        | 0.22          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 8        | 0.22          |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 8        | 0.22          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H   | 21       | 0.22          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H   | 21       | 0.22          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H   | 21       | 0.22          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H   | 25       | 0.22          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H   | 25       | 0.22          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H   | 25       | 0.22          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H   | 28       | 0.22          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H   | 28       | 0.22          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H   | 28       | 0.22          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H   | 30       | 0.22          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H   | 30       | 0.22          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H   | 30       | 0.22          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H   | 32       | 0.22          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H   | 32       | 0.22          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H   | 32       | 0.22          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H   | 11       | 0.22          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H   | 11       | 0.22          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H   | 11       | 0.22          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H   | 16       | 0.22          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H   | 16       | 0.22          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H   | 16       | 0.22          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H   | 18       | 0.22          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H   | 18       | 0.22          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H   | 18       | 0.22          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H   | 20       | 0.22          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H   | 20       | 0.22          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H   | 20       | 0.22          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H   | 23       | 0.22          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H   | 23       | 0.22          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H   | 23       | 0.22          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H   | 27       | 0.22          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H   | 27       | 0.22          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H   | 27       | 0.22          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H   | 29       | 0.22          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H   | 29       | 0.22          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H   | 29       | 0.22          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H   | 33       | 0.22          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H   | 33       | 0.22          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H   | 33       | 0.22          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H   | 35       | 0.22          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H   | 35       | 0.22          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H   | 35       | 0.22          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H   | 40       | 0.22          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H   | 40       | 0.22          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H   | 40       | 0.22          |
| (1,1396) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 16       | 0.22          |
| (1,1396) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 16       | 0.22          |
| (1,1396) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 16       | 0.22          |
| (1,1396) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 29       | 0.22          |
| (1,1396) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 29       | 0.22          |
| (1,1396) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 29       | 0.22          |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 5        | 0.22          |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 5        | 0.22          |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 5        | 0.22          |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 8        | 0.22          |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 8        | 0.22          |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 8        | 0.22          |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 18       | 0.22          |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 18       | 0.22          |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 18       | 0.22          |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 26       | 0.22          |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 26       | 0.22          |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 26       | 0.22          |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 31       | 0.22          |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 31       | 0.22          |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 31       | 0.22          |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 37       | 0.22          |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 37       | 0.22          |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 37       | 0.22          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 23       | 0.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 23       | 0.22          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 23       | 0.22          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 26       | 0.22          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 26       | 0.22          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 26       | 0.22          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 35       | 0.22          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 35       | 0.22          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 35       | 0.22          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 40       | 0.22          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 40       | 0.22          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 40       | 0.22          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 2        | 0.22          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 3        | 0.22          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 4        | 0.22          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 5        | 0.22          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 6        | 0.22          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 7        | 0.22          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 8        | 0.22          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 10       | 0.22          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 11       | 0.22          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 12       | 0.22          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 14       | 0.22          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 15       | 0.22          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 17       | 0.22          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 18       | 0.22          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 19       | 0.22          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 23       | 0.22          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 24       | 0.22          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 25       | 0.22          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 27       | 0.22          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 28       | 0.22          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 29       | 0.22          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 31       | 0.22          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 32       | 0.22          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 33       | 0.22          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 34       | 0.22          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 36       | 0.22          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 37       | 0.22          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 39       | 0.22          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB   | 40       | 0.22          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 11       | 0.22          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 11       | 0.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 11       | 0.22          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 16       | 0.22          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 16       | 0.22          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 16       | 0.22          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 11       | 0.22          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 11       | 0.22          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 11       | 0.22          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 16       | 0.22          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 16       | 0.22          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 16       | 0.22          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 16       | 0.22          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 16       | 0.22          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 16       | 0.22          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 40       | 0.22          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 40       | 0.22          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 40       | 0.22          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 2        | 0.22          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 2        | 0.22          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 2        | 0.22          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 9        | 0.22          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 9        | 0.22          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 9        | 0.22          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 10       | 0.22          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 10       | 0.22          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 10       | 0.22          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 14       | 0.22          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 14       | 0.22          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 14       | 0.22          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 15       | 0.22          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 15       | 0.22          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 15       | 0.22          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 35       | 0.22          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 35       | 0.22          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 35       | 0.22          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 37       | 0.22          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 37       | 0.22          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 37       | 0.22          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 10       | 0.22          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 14       | 0.22          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 16       | 0.22          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 19       | 0.22          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 23       | 0.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 24       | 0.22          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 40       | 0.22          |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 1        | 0.22          |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 25       | 0.22          |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 35       | 0.22          |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 36       | 0.22          |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 39       | 0.22          |
| (1,1184) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 13       | 0.22          |
| (1,1184) | 1:19:A:ILE:H    | 1:97:A:LEU:HA   | 34       | 0.22          |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 2        | 0.22          |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 4        | 0.22          |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 10       | 0.22          |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 13       | 0.22          |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 16       | 0.22          |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 24       | 0.22          |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 29       | 0.22          |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 35       | 0.22          |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 40       | 0.22          |
| (1,1163) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 1        | 0.22          |
| (1,1163) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 2        | 0.22          |
| (1,1163) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 3        | 0.22          |
| (1,1163) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 4        | 0.22          |
| (1,1163) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 8        | 0.22          |
| (1,1163) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 10       | 0.22          |
| (1,1163) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 16       | 0.22          |
| (1,1163) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 20       | 0.22          |
| (1,1163) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 26       | 0.22          |
| (1,1162) | 1:97:A:LEU:H    | 1:29:A:PHE:HE1  | 4        | 0.22          |
| (1,1162) | 1:97:A:LEU:H    | 1:29:A:PHE:HE2  | 4        | 0.22          |
| (1,1162) | 1:97:A:LEU:H    | 1:29:A:PHE:HE1  | 8        | 0.22          |
| (1,1162) | 1:97:A:LEU:H    | 1:29:A:PHE:HE2  | 8        | 0.22          |
| (1,969)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 1        | 0.22          |
| (1,969)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 2        | 0.22          |
| (1,969)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 8        | 0.22          |
| (1,969)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 13       | 0.22          |
| (1,969)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 14       | 0.22          |
| (1,969)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 15       | 0.22          |
| (1,969)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 17       | 0.22          |
| (1,969)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 18       | 0.22          |
| (1,969)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 19       | 0.22          |
| (1,969)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 22       | 0.22          |
| (1,969)  | 1:21:A:VAL:H    | 1:20:A:VAL:HB   | 26       | 0.22          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,969) | 1:21:A:VAL:H | 1:20:A:VAL:HB   | 27       | 0.22          |
| (1,969) | 1:21:A:VAL:H | 1:20:A:VAL:HB   | 28       | 0.22          |
| (1,969) | 1:21:A:VAL:H | 1:20:A:VAL:HB   | 29       | 0.22          |
| (1,969) | 1:21:A:VAL:H | 1:20:A:VAL:HB   | 32       | 0.22          |
| (1,969) | 1:21:A:VAL:H | 1:20:A:VAL:HB   | 33       | 0.22          |
| (1,969) | 1:21:A:VAL:H | 1:20:A:VAL:HB   | 36       | 0.22          |
| (1,969) | 1:21:A:VAL:H | 1:20:A:VAL:HB   | 38       | 0.22          |
| (1,969) | 1:21:A:VAL:H | 1:20:A:VAL:HB   | 39       | 0.22          |
| (1,969) | 1:21:A:VAL:H | 1:20:A:VAL:HB   | 40       | 0.22          |
| (1,932) | 1:98:A:LYS:H | 1:19:A:ILE:HB   | 8        | 0.22          |
| (1,932) | 1:98:A:LYS:H | 1:19:A:ILE:HB   | 21       | 0.22          |
| (1,932) | 1:98:A:LYS:H | 1:19:A:ILE:HB   | 39       | 0.22          |
| (1,919) | 1:37:A:ASP:H | 1:36:A:ASP:HB2  | 1        | 0.22          |
| (1,918) | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 3        | 0.22          |
| (1,918) | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 9        | 0.22          |
| (1,918) | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 12       | 0.22          |
| (1,918) | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 14       | 0.22          |
| (1,918) | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 15       | 0.22          |
| (1,918) | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 21       | 0.22          |
| (1,918) | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 27       | 0.22          |
| (1,888) | 1:80:A:SER:H | 1:43:A:TYR:HB3  | 20       | 0.22          |
| (1,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2   | 7        | 0.22          |
| (1,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2   | 8        | 0.22          |
| (1,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 5        | 0.22          |
| (1,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 40       | 0.22          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 33       | 0.22          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 33       | 0.22          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 33       | 0.22          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 36       | 0.22          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 36       | 0.22          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 36       | 0.22          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 11       | 0.22          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 11       | 0.22          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 11       | 0.22          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 22       | 0.22          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 22       | 0.22          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 22       | 0.22          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 23       | 0.22          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 23       | 0.22          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 23       | 0.22          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 28       | 0.22          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 28       | 0.22          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG23 | 28       | 0.22          |
| (1,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 12       | 0.22          |
| (1,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 14       | 0.22          |
| (1,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 19       | 0.22          |
| (1,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 21       | 0.22          |
| (1,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 29       | 0.22          |
| (1,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 33       | 0.22          |
| (1,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 40       | 0.22          |
| (1,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3  | 10       | 0.22          |
| (1,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3  | 15       | 0.22          |
| (1,685) | 1:23:A:GLU:H  | 1:23:A:GLU:HG3  | 28       | 0.22          |
| (1,685) | 1:23:A:GLU:H  | 1:23:A:GLU:HG3  | 37       | 0.22          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 1        | 0.22          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 3        | 0.22          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 8        | 0.22          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 12       | 0.22          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 13       | 0.22          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 18       | 0.22          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 20       | 0.22          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 23       | 0.22          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 25       | 0.22          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 30       | 0.22          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 38       | 0.22          |
| (1,590) | 1:3:A:ASP:H   | 1:2:A:ILE:HA    | 2        | 0.22          |
| (1,590) | 1:3:A:ASP:H   | 1:2:A:ILE:HA    | 5        | 0.22          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 10       | 0.22          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2  | 10       | 0.22          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 17       | 0.22          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2  | 17       | 0.22          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 27       | 0.22          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2  | 27       | 0.22          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 38       | 0.22          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2  | 38       | 0.22          |
| (1,556) | 1:47:A:THR:H  | 1:48:A:GLU:H    | 4        | 0.22          |
| (1,556) | 1:47:A:THR:H  | 1:48:A:GLU:H    | 5        | 0.22          |
| (1,556) | 1:47:A:THR:H  | 1:48:A:GLU:H    | 11       | 0.22          |
| (1,556) | 1:47:A:THR:H  | 1:48:A:GLU:H    | 16       | 0.22          |
| (1,556) | 1:47:A:THR:H  | 1:48:A:GLU:H    | 31       | 0.22          |
| (1,549) | 1:71:A:VAL:H  | 1:70:A:ASN:HB2  | 31       | 0.22          |
| (1,546) | 1:71:A:VAL:H  | 1:24:A:HIS:HA   | 2        | 0.22          |
| (1,546) | 1:71:A:VAL:H  | 1:24:A:HIS:HA   | 4        | 0.22          |
| (1,546) | 1:71:A:VAL:H  | 1:24:A:HIS:HA   | 11       | 0.22          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 12       | 0.22          |
| (1,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 30       | 0.22          |
| (1,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 32       | 0.22          |
| (1,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 35       | 0.22          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 15       | 0.22          |
| (1,513) | 1:67:A:THR:H | 1:66:A:MET:HG3  | 2        | 0.22          |
| (1,513) | 1:67:A:THR:H | 1:66:A:MET:HG3  | 40       | 0.22          |
| (1,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2  | 4        | 0.22          |
| (1,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2  | 8        | 0.22          |
| (1,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2  | 11       | 0.22          |
| (1,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2  | 12       | 0.22          |
| (1,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2  | 31       | 0.22          |
| (1,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2  | 32       | 0.22          |
| (1,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2  | 33       | 0.22          |
| (1,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2  | 38       | 0.22          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 20       | 0.22          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 23       | 0.22          |
| (1,366) | 1:18:A:ASN:H | 1:18:A:ASN:HB3  | 1        | 0.22          |
| (1,366) | 1:18:A:ASN:H | 1:18:A:ASN:HB3  | 29       | 0.22          |
| (1,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 22       | 0.22          |
| (1,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 23       | 0.22          |
| (1,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 40       | 0.22          |
| (1,248) | 1:95:A:ALA:H | 1:94:A:THR:HB   | 28       | 0.22          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 5        | 0.22          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 5        | 0.22          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 16       | 0.22          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD2  | 16       | 0.22          |
| (1,149) | 1:45:A:GLY:H | 1:46:A:PRO:HD3  | 4        | 0.22          |
| (1,133) | 1:39:A:ILE:H | 1:39:A:ILE:HG13 | 4        | 0.22          |
| (1,133) | 1:39:A:ILE:H | 1:39:A:ILE:HG13 | 5        | 0.22          |
| (1,133) | 1:39:A:ILE:H | 1:39:A:ILE:HG13 | 13       | 0.22          |
| (1,133) | 1:39:A:ILE:H | 1:39:A:ILE:HG13 | 17       | 0.22          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 7        | 0.22          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 13       | 0.22          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 16       | 0.22          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 19       | 0.22          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 21       | 0.22          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 28       | 0.22          |
| (1,129) | 1:39:A:ILE:H | 1:39:A:ILE:HA   | 38       | 0.22          |
| (1,72)  | 1:51:A:GLU:H | 1:50:A:THR:HG21 | 8        | 0.22          |
| (1,72)  | 1:51:A:GLU:H | 1:50:A:THR:HG22 | 8        | 0.22          |
| (1,72)  | 1:51:A:GLU:H | 1:50:A:THR:HG23 | 8        | 0.22          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 11       | 0.22          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 11       | 0.22          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 11       | 0.22          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 12       | 0.22          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 12       | 0.22          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 12       | 0.22          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 24       | 0.22          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 24       | 0.22          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 24       | 0.22          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 27       | 0.22          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 27       | 0.22          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 27       | 0.22          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 30       | 0.22          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 30       | 0.22          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 30       | 0.22          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 34       | 0.22          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 34       | 0.22          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 34       | 0.22          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 39       | 0.22          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 39       | 0.22          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 39       | 0.22          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 11       | 0.21          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 11       | 0.21          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 19       | 0.21          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 19       | 0.21          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 22       | 0.21          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 22       | 0.21          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 40       | 0.21          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 40       | 0.21          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 10       | 0.21          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 11       | 0.21          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 34       | 0.21          |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2  | 30       | 0.21          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2  | 30       | 0.21          |
| (3,3137) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3  | 27       | 0.21          |
| (3,3137) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3  | 27       | 0.21          |
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 10       | 0.21          |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 10       | 0.21          |
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 35       | 0.21          |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 35       | 0.21          |
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 37       | 0.21          |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 37       | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,3055) | 1:57:A:PHE:HB3  | 1:42:A:TRP:HE1  | 13       | 0.21          |
| (3,3055) | 1:57:A:PHE:HB3  | 1:42:A:TRP:HE1  | 37       | 0.21          |
| (3,3019) | 1:30:A:GLU:HB2  | 1:14:A:LYS:HE2  | 11       | 0.21          |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG21 | 15       | 0.21          |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG22 | 15       | 0.21          |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG23 | 15       | 0.21          |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG21 | 22       | 0.21          |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG22 | 22       | 0.21          |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG23 | 22       | 0.21          |
| (3,3004) | 1:15:A:ARG:HG2  | 1:93:A:SER:HB3  | 4        | 0.21          |
| (3,2976) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 8        | 0.21          |
| (3,2976) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 9        | 0.21          |
| (3,2976) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 16       | 0.21          |
| (3,2976) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 17       | 0.21          |
| (3,2976) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 19       | 0.21          |
| (3,2976) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 21       | 0.21          |
| (3,2976) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 22       | 0.21          |
| (3,2976) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 24       | 0.21          |
| (3,2976) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 28       | 0.21          |
| (3,2976) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 39       | 0.21          |
| (3,2976) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 40       | 0.21          |
| (3,2969) | 1:44:A:LYS:HE2  | 1:44:A:LYS:HG2  | 35       | 0.21          |
| (3,2938) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 17       | 0.21          |
| (3,2925) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 37       | 0.21          |
| (3,2886) | 1:102:A:ARG:HD3 | 1:102:A:ARG:HG2 | 3        | 0.21          |
| (3,2886) | 1:102:A:ARG:HD3 | 1:102:A:ARG:HG2 | 5        | 0.21          |
| (3,2886) | 1:102:A:ARG:HD3 | 1:102:A:ARG:HG2 | 8        | 0.21          |
| (3,2886) | 1:102:A:ARG:HD3 | 1:102:A:ARG:HG2 | 11       | 0.21          |
| (3,2886) | 1:102:A:ARG:HD3 | 1:102:A:ARG:HG2 | 23       | 0.21          |
| (3,2886) | 1:102:A:ARG:HD3 | 1:102:A:ARG:HG2 | 29       | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3  | 1:92:A:ARG:HG3  | 2        | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3  | 1:92:A:ARG:HG3  | 3        | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3  | 1:92:A:ARG:HG3  | 4        | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3  | 1:92:A:ARG:HG3  | 5        | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3  | 1:92:A:ARG:HG3  | 6        | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3  | 1:92:A:ARG:HG3  | 7        | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3  | 1:92:A:ARG:HG3  | 8        | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3  | 1:92:A:ARG:HG3  | 11       | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3  | 1:92:A:ARG:HG3  | 12       | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3  | 1:92:A:ARG:HG3  | 15       | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3  | 1:92:A:ARG:HG3  | 16       | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3  | 1:92:A:ARG:HG3  | 17       | 0.21          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,2864) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 19       | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 20       | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 21       | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 22       | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 23       | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 24       | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 25       | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 26       | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 27       | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 28       | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 29       | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 30       | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 31       | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 32       | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 33       | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 34       | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 36       | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 37       | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 39       | 0.21          |
| (3,2864) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 40       | 0.21          |
| (3,2809) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2 | 18       | 0.21          |
| (3,2809) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2 | 20       | 0.21          |
| (3,2809) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2 | 39       | 0.21          |
| (3,2808) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HG2 | 3        | 0.21          |
| (3,2808) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HG2 | 11       | 0.21          |
| (3,2808) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HG2 | 38       | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 1        | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 3        | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 4        | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 6        | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 7        | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 9        | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 10       | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 12       | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 13       | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 14       | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 15       | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 16       | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 17       | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 18       | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 19       | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 20       | 0.21          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 21       | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 22       | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 23       | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 24       | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 25       | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 26       | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 27       | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 28       | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 29       | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 32       | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 34       | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 35       | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 36       | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 37       | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 39       | 0.21          |
| (3,2803) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 40       | 0.21          |
| (3,2761) | 1:90:A:GLU:HB3 | 1:91:A:ALA:H   | 21       | 0.21          |
| (3,2761) | 1:90:A:GLU:HB3 | 1:91:A:ALA:H   | 28       | 0.21          |
| (3,2761) | 1:90:A:GLU:HB3 | 1:91:A:ALA:H   | 32       | 0.21          |
| (3,2761) | 1:90:A:GLU:HB3 | 1:91:A:ALA:H   | 40       | 0.21          |
| (3,2738) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 1        | 0.21          |
| (3,2738) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 4        | 0.21          |
| (3,2738) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 5        | 0.21          |
| (3,2738) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 8        | 0.21          |
| (3,2738) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 9        | 0.21          |
| (3,2738) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 12       | 0.21          |
| (3,2738) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 15       | 0.21          |
| (3,2738) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 16       | 0.21          |
| (3,2738) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 17       | 0.21          |
| (3,2738) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 19       | 0.21          |
| (3,2738) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 21       | 0.21          |
| (3,2738) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 22       | 0.21          |
| (3,2738) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 24       | 0.21          |
| (3,2738) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 27       | 0.21          |
| (3,2738) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 37       | 0.21          |
| (3,2722) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 1        | 0.21          |
| (3,2722) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 16       | 0.21          |
| (3,2722) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 19       | 0.21          |
| (3,2722) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 33       | 0.21          |
| (3,2679) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 7        | 0.21          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 4        | 0.21          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 6        | 0.21          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 7        | 0.21          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 13       | 0.21          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 26       | 0.21          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 29       | 0.21          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 33       | 0.21          |
| (3,2672) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 38       | 0.21          |
| (3,2653) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H   | 5        | 0.21          |
| (3,2653) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H   | 26       | 0.21          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 1        | 0.21          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 4        | 0.21          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 5        | 0.21          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 7        | 0.21          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 9        | 0.21          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 10       | 0.21          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 11       | 0.21          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 12       | 0.21          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 14       | 0.21          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 15       | 0.21          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 16       | 0.21          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 17       | 0.21          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 19       | 0.21          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 20       | 0.21          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 21       | 0.21          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 22       | 0.21          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 23       | 0.21          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 24       | 0.21          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 25       | 0.21          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 29       | 0.21          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 30       | 0.21          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 32       | 0.21          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 34       | 0.21          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 35       | 0.21          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 36       | 0.21          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 37       | 0.21          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 38       | 0.21          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 39       | 0.21          |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 40       | 0.21          |
| (3,2602) | 1:36:A:ASP:HB2 | 1:37:A:ASP:H   | 18       | 0.21          |
| (3,2602) | 1:36:A:ASP:HB2 | 1:37:A:ASP:H   | 29       | 0.21          |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 16       | 0.21          |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 17       | 0.21          |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 23       | 0.21          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 25       | 0.21          |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 26       | 0.21          |
| (3,2554) | 1:92:A:ARG:HA  | 1:83:A:ALA:H   | 34       | 0.21          |
| (3,2554) | 1:92:A:ARG:HA  | 1:83:A:ALA:H   | 38       | 0.21          |
| (3,2538) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 2        | 0.21          |
| (3,2538) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 3        | 0.21          |
| (3,2538) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 6        | 0.21          |
| (3,2538) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 9        | 0.21          |
| (3,2538) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 17       | 0.21          |
| (3,2514) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 10       | 0.21          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 22       | 0.21          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 24       | 0.21          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 25       | 0.21          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 26       | 0.21          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 27       | 0.21          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 30       | 0.21          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 32       | 0.21          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 37       | 0.21          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 38       | 0.21          |
| (3,2485) | 1:9:A:PRO:HD3  | 1:9:A:PRO:HB3  | 23       | 0.21          |
| (3,2434) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 5        | 0.21          |
| (3,2434) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 14       | 0.21          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 5        | 0.21          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 5        | 0.21          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 5        | 0.21          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 14       | 0.21          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 14       | 0.21          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 14       | 0.21          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 30       | 0.21          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 30       | 0.21          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 30       | 0.21          |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 2        | 0.21          |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 8        | 0.21          |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 12       | 0.21          |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 19       | 0.21          |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 33       | 0.21          |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 35       | 0.21          |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 20       | 0.21          |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 21       | 0.21          |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 29       | 0.21          |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 31       | 0.21          |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 33       | 0.21          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2289) | 1:96:A:GLU:HG2  | 1:97:A:LEU:H   | 35       | 0.21          |
| (3,2289) | 1:96:A:GLU:HG2  | 1:97:A:LEU:H   | 39       | 0.21          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1 | 5        | 0.21          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2 | 5        | 0.21          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1 | 13       | 0.21          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2 | 13       | 0.21          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1 | 17       | 0.21          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2 | 17       | 0.21          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1 | 21       | 0.21          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2 | 21       | 0.21          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1 | 33       | 0.21          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2 | 33       | 0.21          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1 | 35       | 0.21          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2 | 35       | 0.21          |
| (3,2239) | 1:18:A:ASN:HB3  | 1:18:A:ASN:H   | 2        | 0.21          |
| (3,2239) | 1:18:A:ASN:HB3  | 1:18:A:ASN:H   | 14       | 0.21          |
| (3,2239) | 1:18:A:ASN:HB3  | 1:18:A:ASN:H   | 17       | 0.21          |
| (3,2239) | 1:18:A:ASN:HB3  | 1:18:A:ASN:H   | 18       | 0.21          |
| (3,2239) | 1:18:A:ASN:HB3  | 1:18:A:ASN:H   | 21       | 0.21          |
| (3,2239) | 1:18:A:ASN:HB3  | 1:18:A:ASN:H   | 30       | 0.21          |
| (3,2239) | 1:18:A:ASN:HB3  | 1:18:A:ASN:H   | 33       | 0.21          |
| (3,2239) | 1:18:A:ASN:HB3  | 1:18:A:ASN:H   | 34       | 0.21          |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H   | 3        | 0.21          |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H   | 14       | 0.21          |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H   | 15       | 0.21          |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H   | 26       | 0.21          |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H   | 29       | 0.21          |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H   | 34       | 0.21          |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H   | 40       | 0.21          |
| (3,2132) | 1:47:A:THR:HG21 | 1:47:A:THR:HB  | 5        | 0.21          |
| (3,2132) | 1:47:A:THR:HG22 | 1:47:A:THR:HB  | 5        | 0.21          |
| (3,2132) | 1:47:A:THR:HG23 | 1:47:A:THR:HB  | 5        | 0.21          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 1        | 0.21          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 1        | 0.21          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 1        | 0.21          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 8        | 0.21          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 8        | 0.21          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 8        | 0.21          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 8        | 0.21          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 8        | 0.21          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 8        | 0.21          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 9        | 0.21          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 9        | 0.21          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 9        | 0.21          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 9        | 0.21          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 9        | 0.21          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 9        | 0.21          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 13       | 0.21          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 13       | 0.21          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 13       | 0.21          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 13       | 0.21          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 13       | 0.21          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 13       | 0.21          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 3        | 0.21          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 3        | 0.21          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 3        | 0.21          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 6        | 0.21          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 6        | 0.21          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 6        | 0.21          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 10       | 0.21          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 10       | 0.21          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 10       | 0.21          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 27       | 0.21          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 27       | 0.21          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 27       | 0.21          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 33       | 0.21          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 33       | 0.21          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 33       | 0.21          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 6        | 0.21          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 6        | 0.21          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 6        | 0.21          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 9        | 0.21          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 9        | 0.21          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 9        | 0.21          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 10       | 0.21          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 10       | 0.21          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 10       | 0.21          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 15       | 0.21          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 15       | 0.21          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 15       | 0.21          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 16       | 0.21          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 16       | 0.21          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 16       | 0.21          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 17       | 0.21          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 17       | 0.21          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 17       | 0.21          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 20       | 0.21          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 20       | 0.21          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 20       | 0.21          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 21       | 0.21          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 21       | 0.21          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 21       | 0.21          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 24       | 0.21          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 24       | 0.21          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 24       | 0.21          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 29       | 0.21          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 29       | 0.21          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 29       | 0.21          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 33       | 0.21          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 33       | 0.21          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 33       | 0.21          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 39       | 0.21          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 39       | 0.21          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 39       | 0.21          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA  | 19       | 0.21          |
| (3,1938) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 4        | 0.21          |
| (3,1938) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 10       | 0.21          |
| (3,1938) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2 | 15       | 0.21          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 5        | 0.21          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 9        | 0.21          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 10       | 0.21          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 11       | 0.21          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 18       | 0.21          |
| (3,1919) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2 | 22       | 0.21          |
| (3,1907) | 1:66:A:MET:HE1  | 1:43:A:TYR:H   | 2        | 0.21          |
| (3,1907) | 1:66:A:MET:HE2  | 1:43:A:TYR:H   | 2        | 0.21          |
| (3,1907) | 1:66:A:MET:HE3  | 1:43:A:TYR:H   | 2        | 0.21          |
| (3,1907) | 1:66:A:MET:HE1  | 1:43:A:TYR:H   | 6        | 0.21          |
| (3,1907) | 1:66:A:MET:HE2  | 1:43:A:TYR:H   | 6        | 0.21          |
| (3,1907) | 1:66:A:MET:HE3  | 1:43:A:TYR:H   | 6        | 0.21          |
| (3,1907) | 1:66:A:MET:HE1  | 1:43:A:TYR:H   | 7        | 0.21          |
| (3,1907) | 1:66:A:MET:HE2  | 1:43:A:TYR:H   | 7        | 0.21          |
| (3,1907) | 1:66:A:MET:HE3  | 1:43:A:TYR:H   | 7        | 0.21          |
| (3,1907) | 1:66:A:MET:HE1  | 1:43:A:TYR:H   | 40       | 0.21          |
| (3,1907) | 1:66:A:MET:HE2  | 1:43:A:TYR:H   | 40       | 0.21          |
| (3,1907) | 1:66:A:MET:HE3  | 1:43:A:TYR:H   | 40       | 0.21          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,1828) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 1        | 0.21          |
| (3,1828) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 5        | 0.21          |
| (3,1828) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 6        | 0.21          |
| (3,1828) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 7        | 0.21          |
| (3,1828) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 10       | 0.21          |
| (3,1828) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 21       | 0.21          |
| (3,1828) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 23       | 0.21          |
| (3,1828) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 24       | 0.21          |
| (3,1828) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 25       | 0.21          |
| (3,1828) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 26       | 0.21          |
| (3,1828) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 30       | 0.21          |
| (3,1828) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 32       | 0.21          |
| (3,1828) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 33       | 0.21          |
| (3,1828) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 34       | 0.21          |
| (3,1828) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 35       | 0.21          |
| (3,1828) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 36       | 0.21          |
| (3,1828) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 39       | 0.21          |
| (3,1828) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 40       | 0.21          |
| (3,1815) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 1        | 0.21          |
| (3,1815) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 5        | 0.21          |
| (3,1815) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 6        | 0.21          |
| (3,1815) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 7        | 0.21          |
| (3,1815) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 10       | 0.21          |
| (3,1815) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 21       | 0.21          |
| (3,1815) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 23       | 0.21          |
| (3,1815) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 24       | 0.21          |
| (3,1815) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 25       | 0.21          |
| (3,1815) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 26       | 0.21          |
| (3,1815) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 30       | 0.21          |
| (3,1815) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 32       | 0.21          |
| (3,1815) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 33       | 0.21          |
| (3,1815) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 34       | 0.21          |
| (3,1815) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 35       | 0.21          |
| (3,1815) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 36       | 0.21          |
| (3,1815) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 39       | 0.21          |
| (3,1815) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 40       | 0.21          |
| (3,1781) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 25       | 0.21          |
| (3,1781) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 27       | 0.21          |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 1        | 0.21          |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 4        | 0.21          |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 8        | 0.21          |
| (3,1731) | 1:48:A:GLU:HB2 | 1:48:A:GLU:H   | 12       | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1731) | 1:48:A:GLU:HB2  | 1:48:A:GLU:H    | 18       | 0.21          |
| (3,1731) | 1:48:A:GLU:HB2  | 1:48:A:GLU:H    | 19       | 0.21          |
| (3,1731) | 1:48:A:GLU:HB2  | 1:48:A:GLU:H    | 29       | 0.21          |
| (3,1721) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG11 | 36       | 0.21          |
| (3,1721) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG12 | 36       | 0.21          |
| (3,1721) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG13 | 36       | 0.21          |
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG11 | 36       | 0.21          |
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG12 | 36       | 0.21          |
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 36       | 0.21          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 36       | 0.21          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 36       | 0.21          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 36       | 0.21          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 14       | 0.21          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 14       | 0.21          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 14       | 0.21          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 4        | 0.21          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 4        | 0.21          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 4        | 0.21          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 4        | 0.21          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 4        | 0.21          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 4        | 0.21          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 4        | 0.21          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 4        | 0.21          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 4        | 0.21          |
| (3,1628) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2  | 21       | 0.21          |
| (3,1628) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2  | 21       | 0.21          |
| (3,1628) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2  | 21       | 0.21          |
| (3,1628) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2  | 32       | 0.21          |
| (3,1628) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2  | 32       | 0.21          |
| (3,1628) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2  | 32       | 0.21          |
| (3,1628) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2  | 34       | 0.21          |
| (3,1628) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2  | 34       | 0.21          |
| (3,1628) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2  | 34       | 0.21          |
| (3,1628) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2  | 39       | 0.21          |
| (3,1628) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2  | 39       | 0.21          |
| (3,1628) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2  | 39       | 0.21          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 3        | 0.21          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 3        | 0.21          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 3        | 0.21          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 4        | 0.21          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 4        | 0.21          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 4        | 0.21          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2 | 7        | 0.21          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 7        | 0.21          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 7        | 0.21          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2 | 25       | 0.21          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 25       | 0.21          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 25       | 0.21          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2 | 33       | 0.21          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 33       | 0.21          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 33       | 0.21          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2 | 37       | 0.21          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 37       | 0.21          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 37       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB  | 1        | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB  | 1        | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB  | 1        | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB  | 3        | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB  | 3        | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB  | 3        | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB  | 4        | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB  | 4        | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB  | 4        | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB  | 5        | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB  | 5        | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB  | 5        | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB  | 6        | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB  | 6        | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB  | 6        | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB  | 7        | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB  | 7        | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB  | 7        | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB  | 8        | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB  | 8        | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB  | 8        | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB  | 9        | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB  | 9        | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB  | 9        | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB  | 10       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB  | 10       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB  | 10       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB  | 12       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB  | 12       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB  | 12       | 0.21          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 13       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 13       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 13       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 14       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 14       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 14       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 15       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 15       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 15       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 16       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 16       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 16       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 17       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 17       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 17       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 18       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 18       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 18       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 19       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 19       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 19       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 20       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 20       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 20       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 21       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 21       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 21       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 22       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 22       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 22       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 23       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 23       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 23       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 25       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 25       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 25       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 26       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 26       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 26       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 27       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 27       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 27       | 0.21          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 28       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 28       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 28       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 29       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 29       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 29       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 30       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 30       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 30       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 31       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 31       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 31       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 32       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 32       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 32       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 33       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 33       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 33       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 34       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 34       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 34       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 35       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 35       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 35       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 37       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 37       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 37       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 39       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 39       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 39       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 40       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 40       | 0.21          |
| (3,1584) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 40       | 0.21          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA | 4        | 0.21          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA | 4        | 0.21          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA | 4        | 0.21          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA | 6        | 0.21          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA | 6        | 0.21          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA | 6        | 0.21          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA | 29       | 0.21          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA | 29       | 0.21          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA | 29       | 0.21          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 37       | 0.21          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 37       | 0.21          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 37       | 0.21          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 9        | 0.21          |
| (3,1486) | 1:81:A:VAL:HB   | 1:82:A:ILE:H   | 20       | 0.21          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 6        | 0.21          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 6        | 0.21          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 6        | 0.21          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 11       | 0.21          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 11       | 0.21          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 11       | 0.21          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 15       | 0.21          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 15       | 0.21          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 15       | 0.21          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 16       | 0.21          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 16       | 0.21          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 16       | 0.21          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 17       | 0.21          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 17       | 0.21          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 17       | 0.21          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 20       | 0.21          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 20       | 0.21          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 20       | 0.21          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 26       | 0.21          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 26       | 0.21          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 26       | 0.21          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 40       | 0.21          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 40       | 0.21          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 40       | 0.21          |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 17       | 0.21          |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 17       | 0.21          |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 17       | 0.21          |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 21       | 0.21          |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 21       | 0.21          |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 21       | 0.21          |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 24       | 0.21          |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 24       | 0.21          |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 24       | 0.21          |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 34       | 0.21          |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 34       | 0.21          |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 34       | 0.21          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 9        | 0.21          |

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| Key      | Atom-1          | Atom-2       | Model ID | Violation (Å) |
|----------|-----------------|--------------|----------|---------------|
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H | 9        | 0.21          |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H | 9        | 0.21          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H | 14       | 0.21          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H | 14       | 0.21          |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H | 14       | 0.21          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H | 15       | 0.21          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H | 15       | 0.21          |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H | 15       | 0.21          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H | 22       | 0.21          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H | 22       | 0.21          |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H | 22       | 0.21          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 3        | 0.21          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 3        | 0.21          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 3        | 0.21          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 19       | 0.21          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 19       | 0.21          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 19       | 0.21          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 36       | 0.21          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 36       | 0.21          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 36       | 0.21          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 40       | 0.21          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 40       | 0.21          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 40       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 2        | 0.21          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 2        | 0.21          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 2        | 0.21          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 4        | 0.21          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 4        | 0.21          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 4        | 0.21          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 5        | 0.21          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 5        | 0.21          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 5        | 0.21          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 7        | 0.21          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 7        | 0.21          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 7        | 0.21          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 8        | 0.21          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 8        | 0.21          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 8        | 0.21          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 10       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 10       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 10       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 13       | 0.21          |

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| Key      | Atom-1          | Atom-2       | Model ID | Violation (Å) |
|----------|-----------------|--------------|----------|---------------|
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 13       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 13       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 14       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 14       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 14       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 15       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 15       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 15       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 17       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 17       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 17       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 21       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 21       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 21       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 22       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 22       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 22       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 24       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 24       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 24       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 25       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 25       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 25       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 26       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 26       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 26       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 28       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 28       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 28       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 30       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 30       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 30       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 31       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 31       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 31       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 32       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 32       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 32       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 34       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 34       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 34       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 36       | 0.21          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H   | 36       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H   | 36       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H   | 37       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H   | 37       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H   | 37       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H   | 38       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H   | 38       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H   | 38       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H   | 39       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H   | 39       | 0.21          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H   | 39       | 0.21          |
| (3,1400) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 4        | 0.21          |
| (3,1400) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 4        | 0.21          |
| (3,1400) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 4        | 0.21          |
| (3,1400) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 6        | 0.21          |
| (3,1400) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 6        | 0.21          |
| (3,1400) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 6        | 0.21          |
| (3,1400) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 9        | 0.21          |
| (3,1400) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 9        | 0.21          |
| (3,1400) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 9        | 0.21          |
| (3,1400) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 12       | 0.21          |
| (3,1400) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 12       | 0.21          |
| (3,1400) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 12       | 0.21          |
| (3,1400) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 17       | 0.21          |
| (3,1400) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 17       | 0.21          |
| (3,1400) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 17       | 0.21          |
| (3,1400) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 19       | 0.21          |
| (3,1400) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 19       | 0.21          |
| (3,1400) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 19       | 0.21          |
| (3,1400) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 20       | 0.21          |
| (3,1400) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 20       | 0.21          |
| (3,1400) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 20       | 0.21          |
| (3,1400) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 38       | 0.21          |
| (3,1400) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 38       | 0.21          |
| (3,1400) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 38       | 0.21          |
| (3,1400) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 40       | 0.21          |
| (3,1400) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 40       | 0.21          |
| (3,1400) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 40       | 0.21          |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3 | 18       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 1        | 0.21          |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 1        | 0.21          |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 1        | 0.21          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 3        | 0.21          |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 3        | 0.21          |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 3        | 0.21          |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 11       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 11       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 11       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 14       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 14       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 14       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 15       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 15       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 15       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 17       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 17       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 17       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 19       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 19       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 19       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 22       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 22       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 22       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 23       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 23       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 23       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 25       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 25       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 25       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 33       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 33       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 33       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 34       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 34       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 34       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 35       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 35       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 35       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 36       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 36       | 0.21          |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 36       | 0.21          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 3        | 0.21          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 3        | 0.21          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 3        | 0.21          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 7        | 0.21          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 7        | 0.21          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 7        | 0.21          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 17       | 0.21          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 17       | 0.21          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 17       | 0.21          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 18       | 0.21          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 18       | 0.21          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 18       | 0.21          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 19       | 0.21          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 19       | 0.21          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 19       | 0.21          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 25       | 0.21          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 25       | 0.21          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 25       | 0.21          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 30       | 0.21          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 30       | 0.21          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 30       | 0.21          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 38       | 0.21          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 38       | 0.21          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 38       | 0.21          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 1        | 0.21          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 9        | 0.21          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 13       | 0.21          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 16       | 0.21          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 20       | 0.21          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 21       | 0.21          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 22       | 0.21          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 26       | 0.21          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 30       | 0.21          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 35       | 0.21          |
| (3,1335) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 38       | 0.21          |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA  | 3        | 0.21          |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA  | 3        | 0.21          |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA  | 3        | 0.21          |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA  | 7        | 0.21          |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA  | 7        | 0.21          |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA  | 7        | 0.21          |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA  | 10       | 0.21          |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA  | 10       | 0.21          |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA  | 10       | 0.21          |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA  | 11       | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 11       | 0.21          |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 11       | 0.21          |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 14       | 0.21          |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 14       | 0.21          |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 14       | 0.21          |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 19       | 0.21          |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 19       | 0.21          |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 19       | 0.21          |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 20       | 0.21          |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 20       | 0.21          |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 20       | 0.21          |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 26       | 0.21          |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 26       | 0.21          |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 26       | 0.21          |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 27       | 0.21          |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 27       | 0.21          |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 27       | 0.21          |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 40       | 0.21          |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 40       | 0.21          |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 40       | 0.21          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 24       | 0.21          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 24       | 0.21          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 24       | 0.21          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 24       | 0.21          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 24       | 0.21          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 24       | 0.21          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 8        | 0.21          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 8        | 0.21          |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 8        | 0.21          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 9        | 0.21          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 9        | 0.21          |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 9        | 0.21          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 27       | 0.21          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 27       | 0.21          |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 27       | 0.21          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 8        | 0.21          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 8        | 0.21          |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 8        | 0.21          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 9        | 0.21          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 9        | 0.21          |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 9        | 0.21          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 27       | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 27       | 0.21          |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 27       | 0.21          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 4        | 0.21          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 4        | 0.21          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 4        | 0.21          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 27       | 0.21          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 27       | 0.21          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 27       | 0.21          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 28       | 0.21          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 28       | 0.21          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 28       | 0.21          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 2        | 0.21          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 5        | 0.21          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 8        | 0.21          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 13       | 0.21          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 15       | 0.21          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 17       | 0.21          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 18       | 0.21          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 21       | 0.21          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 25       | 0.21          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 27       | 0.21          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 28       | 0.21          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 30       | 0.21          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 31       | 0.21          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 32       | 0.21          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 33       | 0.21          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 34       | 0.21          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 35       | 0.21          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 36       | 0.21          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 37       | 0.21          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 38       | 0.21          |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 16       | 0.21          |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 18       | 0.21          |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 19       | 0.21          |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 22       | 0.21          |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 23       | 0.21          |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 37       | 0.21          |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 38       | 0.21          |
| (3,1180) | 1:47:A:THR:H    | 1:44:A:LYS:HB3  | 5        | 0.21          |
| (3,1173) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 3        | 0.21          |
| (3,1173) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 6        | 0.21          |
| (3,1173) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 12       | 0.21          |

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| Key      | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|----------|---------------|----------------|----------|---------------|
| (3,1173) | 1:14:A:LYS:H  | 1:14:A:LYS:HD2 | 14       | 0.21          |
| (3,1173) | 1:14:A:LYS:H  | 1:14:A:LYS:HD2 | 15       | 0.21          |
| (3,1173) | 1:14:A:LYS:H  | 1:14:A:LYS:HD2 | 18       | 0.21          |
| (3,1173) | 1:14:A:LYS:H  | 1:14:A:LYS:HD2 | 21       | 0.21          |
| (3,1173) | 1:14:A:LYS:H  | 1:14:A:LYS:HD2 | 33       | 0.21          |
| (3,1173) | 1:14:A:LYS:H  | 1:14:A:LYS:HD2 | 38       | 0.21          |
| (3,1167) | 1:75:A:ASP:H  | 1:74:A:ASP:HB2 | 9        | 0.21          |
| (3,1167) | 1:75:A:ASP:H  | 1:74:A:ASP:HB2 | 13       | 0.21          |
| (3,1167) | 1:75:A:ASP:H  | 1:74:A:ASP:HB2 | 19       | 0.21          |
| (3,1167) | 1:75:A:ASP:H  | 1:74:A:ASP:HB2 | 30       | 0.21          |
| (3,1167) | 1:75:A:ASP:H  | 1:74:A:ASP:HB2 | 32       | 0.21          |
| (3,1167) | 1:75:A:ASP:H  | 1:74:A:ASP:HB2 | 34       | 0.21          |
| (3,1167) | 1:75:A:ASP:H  | 1:74:A:ASP:HB2 | 38       | 0.21          |
| (3,1167) | 1:75:A:ASP:H  | 1:74:A:ASP:HB2 | 39       | 0.21          |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 19       | 0.21          |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 21       | 0.21          |
| (3,1003) | 1:5:A:PHE:H   | 1:4:A:PRO:HA   | 20       | 0.21          |
| (3,970)  | 1:21:A:VAL:H  | 1:20:A:VAL:HB  | 4        | 0.21          |
| (3,970)  | 1:21:A:VAL:H  | 1:20:A:VAL:HB  | 11       | 0.21          |
| (3,970)  | 1:21:A:VAL:H  | 1:20:A:VAL:HB  | 12       | 0.21          |
| (3,970)  | 1:21:A:VAL:H  | 1:20:A:VAL:HB  | 21       | 0.21          |
| (3,970)  | 1:21:A:VAL:H  | 1:20:A:VAL:HB  | 24       | 0.21          |
| (3,970)  | 1:21:A:VAL:H  | 1:20:A:VAL:HB  | 25       | 0.21          |
| (3,970)  | 1:21:A:VAL:H  | 1:20:A:VAL:HB  | 30       | 0.21          |
| (3,970)  | 1:21:A:VAL:H  | 1:20:A:VAL:HB  | 31       | 0.21          |
| (3,970)  | 1:21:A:VAL:H  | 1:20:A:VAL:HB  | 37       | 0.21          |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB  | 9        | 0.21          |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB  | 15       | 0.21          |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB  | 34       | 0.21          |
| (3,920)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB2 | 18       | 0.21          |
| (3,920)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB2 | 29       | 0.21          |
| (3,919)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB3 | 16       | 0.21          |
| (3,919)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB3 | 17       | 0.21          |
| (3,919)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB3 | 23       | 0.21          |
| (3,919)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB3 | 25       | 0.21          |
| (3,919)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB3 | 26       | 0.21          |
| (3,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3  | 32       | 0.21          |
| (3,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3  | 35       | 0.21          |
| (3,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3  | 37       | 0.21          |
| (3,870)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD2  | 4        | 0.21          |
| (3,870)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD2  | 6        | 0.21          |
| (3,870)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD2  | 14       | 0.21          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (3,870) | 1:8:A:GLU:H   | 1:9:A:PRO:HD2   | 18       | 0.21          |
| (3,870) | 1:8:A:GLU:H   | 1:9:A:PRO:HD2   | 20       | 0.21          |
| (3,870) | 1:8:A:GLU:H   | 1:9:A:PRO:HD2   | 30       | 0.21          |
| (3,869) | 1:8:A:GLU:H   | 1:7:A:ALA:HA    | 20       | 0.21          |
| (3,849) | 1:83:A:ALA:H  | 1:91:A:ALA:HB1  | 7        | 0.21          |
| (3,849) | 1:83:A:ALA:H  | 1:91:A:ALA:HB2  | 7        | 0.21          |
| (3,849) | 1:83:A:ALA:H  | 1:91:A:ALA:HB3  | 7        | 0.21          |
| (3,849) | 1:83:A:ALA:H  | 1:91:A:ALA:HB1  | 12       | 0.21          |
| (3,849) | 1:83:A:ALA:H  | 1:91:A:ALA:HB2  | 12       | 0.21          |
| (3,849) | 1:83:A:ALA:H  | 1:91:A:ALA:HB3  | 12       | 0.21          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG21 | 3        | 0.21          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG22 | 3        | 0.21          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG23 | 3        | 0.21          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG21 | 9        | 0.21          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG22 | 9        | 0.21          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG23 | 9        | 0.21          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG21 | 14       | 0.21          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG22 | 14       | 0.21          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG23 | 14       | 0.21          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG21 | 24       | 0.21          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG22 | 24       | 0.21          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG23 | 24       | 0.21          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG21 | 32       | 0.21          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG22 | 32       | 0.21          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG23 | 32       | 0.21          |
| (3,801) | 1:54:A:LYS:H  | 1:54:A:LYS:HD2  | 17       | 0.21          |
| (3,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 4        | 0.21          |
| (3,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 13       | 0.21          |
| (3,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 15       | 0.21          |
| (3,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 16       | 0.21          |
| (3,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 18       | 0.21          |
| (3,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 20       | 0.21          |
| (3,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 25       | 0.21          |
| (3,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 28       | 0.21          |
| (3,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 30       | 0.21          |
| (3,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 31       | 0.21          |
| (3,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 34       | 0.21          |
| (3,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 37       | 0.21          |
| (3,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 38       | 0.21          |
| (3,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 39       | 0.21          |
| (3,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 8        | 0.21          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 10       | 0.21          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3 | 11       | 0.21          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3 | 19       | 0.21          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3 | 27       | 0.21          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3 | 28       | 0.21          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3 | 39       | 0.21          |
| (3,590) | 1:3:A:ASP:H   | 1:2:A:ILE:HA   | 10       | 0.21          |
| (3,590) | 1:3:A:ASP:H   | 1:2:A:ILE:HA   | 12       | 0.21          |
| (3,590) | 1:3:A:ASP:H   | 1:2:A:ILE:HA   | 14       | 0.21          |
| (3,590) | 1:3:A:ASP:H   | 1:2:A:ILE:HA   | 17       | 0.21          |
| (3,590) | 1:3:A:ASP:H   | 1:2:A:ILE:HA   | 19       | 0.21          |
| (3,590) | 1:3:A:ASP:H   | 1:2:A:ILE:HA   | 28       | 0.21          |
| (3,589) | 1:93:A:SER:H  | 1:92:A:ARG:HG2 | 18       | 0.21          |
| (3,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1 | 6        | 0.21          |
| (3,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2 | 6        | 0.21          |
| (3,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1 | 16       | 0.21          |
| (3,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2 | 16       | 0.21          |
| (3,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1 | 28       | 0.21          |
| (3,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2 | 28       | 0.21          |
| (3,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1 | 29       | 0.21          |
| (3,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2 | 29       | 0.21          |
| (3,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1 | 37       | 0.21          |
| (3,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2 | 37       | 0.21          |
| (3,556) | 1:47:A:THR:H  | 1:48:A:GLU:H   | 6        | 0.21          |
| (3,556) | 1:47:A:THR:H  | 1:48:A:GLU:H   | 8        | 0.21          |
| (3,556) | 1:47:A:THR:H  | 1:48:A:GLU:H   | 10       | 0.21          |
| (3,556) | 1:47:A:THR:H  | 1:48:A:GLU:H   | 19       | 0.21          |
| (3,556) | 1:47:A:THR:H  | 1:48:A:GLU:H   | 26       | 0.21          |
| (3,556) | 1:47:A:THR:H  | 1:48:A:GLU:H   | 28       | 0.21          |
| (3,556) | 1:47:A:THR:H  | 1:48:A:GLU:H   | 29       | 0.21          |
| (3,556) | 1:47:A:THR:H  | 1:48:A:GLU:H   | 37       | 0.21          |
| (3,556) | 1:47:A:THR:H  | 1:48:A:GLU:H   | 38       | 0.21          |
| (3,549) | 1:71:A:VAL:H  | 1:70:A:ASN:HB2 | 4        | 0.21          |
| (3,549) | 1:71:A:VAL:H  | 1:70:A:ASN:HB2 | 13       | 0.21          |
| (3,549) | 1:71:A:VAL:H  | 1:70:A:ASN:HB2 | 16       | 0.21          |
| (3,549) | 1:71:A:VAL:H  | 1:70:A:ASN:HB2 | 35       | 0.21          |
| (3,549) | 1:71:A:VAL:H  | 1:70:A:ASN:HB2 | 37       | 0.21          |
| (3,546) | 1:71:A:VAL:H  | 1:24:A:HIS:HA  | 31       | 0.21          |
| (3,529) | 1:99:A:GLY:H  | 1:76:A:GLU:HB2 | 34       | 0.21          |
| (3,525) | 1:99:A:GLY:H  | 1:100:A:GLU:H  | 9        | 0.21          |
| (3,525) | 1:99:A:GLY:H  | 1:100:A:GLU:H  | 34       | 0.21          |
| (3,513) | 1:67:A:THR:H  | 1:66:A:MET:HG3 | 21       | 0.21          |
| (3,513) | 1:67:A:THR:H  | 1:66:A:MET:HG3 | 24       | 0.21          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (3,513) | 1:67:A:THR:H  | 1:66:A:MET:HG3  | 33       | 0.21          |
| (3,423) | 1:69:A:HIS:H  | 1:69:A:HIS:HD2  | 2        | 0.21          |
| (3,423) | 1:69:A:HIS:H  | 1:69:A:HIS:HD2  | 3        | 0.21          |
| (3,423) | 1:69:A:HIS:H  | 1:69:A:HIS:HD2  | 19       | 0.21          |
| (3,423) | 1:69:A:HIS:H  | 1:69:A:HIS:HD2  | 20       | 0.21          |
| (3,423) | 1:69:A:HIS:H  | 1:69:A:HIS:HD2  | 36       | 0.21          |
| (3,423) | 1:69:A:HIS:H  | 1:69:A:HIS:HD2  | 37       | 0.21          |
| (3,416) | 1:96:A:GLU:H  | 1:96:A:GLU:HB3  | 28       | 0.21          |
| (3,394) | 1:77:A:GLY:H  | 1:97:A:LEU:HA   | 21       | 0.21          |
| (3,394) | 1:77:A:GLY:H  | 1:97:A:LEU:HA   | 31       | 0.21          |
| (3,394) | 1:77:A:GLY:H  | 1:97:A:LEU:HA   | 39       | 0.21          |
| (3,369) | 1:18:A:ASN:H  | 1:17:A:GLN:HB2  | 5        | 0.21          |
| (3,369) | 1:18:A:ASN:H  | 1:17:A:GLN:HB2  | 26       | 0.21          |
| (3,366) | 1:18:A:ASN:H  | 1:18:A:ASN:HB3  | 2        | 0.21          |
| (3,366) | 1:18:A:ASN:H  | 1:18:A:ASN:HB3  | 14       | 0.21          |
| (3,366) | 1:18:A:ASN:H  | 1:18:A:ASN:HB3  | 17       | 0.21          |
| (3,366) | 1:18:A:ASN:H  | 1:18:A:ASN:HB3  | 18       | 0.21          |
| (3,366) | 1:18:A:ASN:H  | 1:18:A:ASN:HB3  | 21       | 0.21          |
| (3,366) | 1:18:A:ASN:H  | 1:18:A:ASN:HB3  | 30       | 0.21          |
| (3,366) | 1:18:A:ASN:H  | 1:18:A:ASN:HB3  | 33       | 0.21          |
| (3,366) | 1:18:A:ASN:H  | 1:18:A:ASN:HB3  | 34       | 0.21          |
| (3,343) | 1:14:A:LYS:H  | 1:33:A:VAL:HA   | 4        | 0.21          |
| (3,343) | 1:14:A:LYS:H  | 1:33:A:VAL:HA   | 11       | 0.21          |
| (3,343) | 1:14:A:LYS:H  | 1:33:A:VAL:HA   | 19       | 0.21          |
| (3,343) | 1:14:A:LYS:H  | 1:33:A:VAL:HA   | 25       | 0.21          |
| (3,343) | 1:14:A:LYS:H  | 1:33:A:VAL:HA   | 26       | 0.21          |
| (3,343) | 1:14:A:LYS:H  | 1:33:A:VAL:HA   | 39       | 0.21          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 8        | 0.21          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 8        | 0.21          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 8        | 0.21          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 9        | 0.21          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 9        | 0.21          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 9        | 0.21          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 27       | 0.21          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 27       | 0.21          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 27       | 0.21          |
| (3,176) | 1:10:A:ILE:H  | 1:35:A:PHE:HD1  | 23       | 0.21          |
| (3,176) | 1:10:A:ILE:H  | 1:35:A:PHE:HD2  | 23       | 0.21          |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 19       | 0.21          |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 21       | 0.21          |
| (3,135) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 10       | 0.21          |
| (3,135) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 12       | 0.21          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,135)  | 1:39:A:ILE:H   | 1:39:A:ILE:HG13 | 35       | 0.21          |
| (3,135)  | 1:39:A:ILE:H   | 1:39:A:ILE:HG13 | 40       | 0.21          |
| (3,102)  | 1:22:A:SER:H   | 1:21:A:VAL:HB   | 8        | 0.21          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 1        | 0.21          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 1        | 0.21          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 1        | 0.21          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 2        | 0.21          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 2        | 0.21          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 2        | 0.21          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 5        | 0.21          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 5        | 0.21          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 5        | 0.21          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 9        | 0.21          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 9        | 0.21          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 9        | 0.21          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 15       | 0.21          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 15       | 0.21          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 15       | 0.21          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 17       | 0.21          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 17       | 0.21          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 17       | 0.21          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 26       | 0.21          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 26       | 0.21          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 26       | 0.21          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 28       | 0.21          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 28       | 0.21          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 28       | 0.21          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 29       | 0.21          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 29       | 0.21          |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 29       | 0.21          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 11       | 0.21          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 11       | 0.21          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 19       | 0.21          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 19       | 0.21          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 22       | 0.21          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 22       | 0.21          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 40       | 0.21          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 40       | 0.21          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 10       | 0.21          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 11       | 0.21          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 34       | 0.21          |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2  | 30       | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3134) | 1:65:A:TYR:HE2  | 1:30:A:GLU:HB2  | 30       | 0.21          |
| (1,3131) | 1:65:A:TYR:HE1  | 1:63:A:CYS:HB3  | 27       | 0.21          |
| (1,3131) | 1:65:A:TYR:HE2  | 1:63:A:CYS:HB3  | 27       | 0.21          |
| (1,3127) | 1:55:A:TYR:HD1  | 1:49:A:LEU:HB2  | 10       | 0.21          |
| (1,3127) | 1:55:A:TYR:HD2  | 1:49:A:LEU:HB2  | 10       | 0.21          |
| (1,3127) | 1:55:A:TYR:HD1  | 1:49:A:LEU:HB2  | 35       | 0.21          |
| (1,3127) | 1:55:A:TYR:HD2  | 1:49:A:LEU:HB2  | 35       | 0.21          |
| (1,3127) | 1:55:A:TYR:HD1  | 1:49:A:LEU:HB2  | 37       | 0.21          |
| (1,3127) | 1:55:A:TYR:HD2  | 1:49:A:LEU:HB2  | 37       | 0.21          |
| (1,3047) | 1:57:A:PHE:HB3  | 1:42:A:TRP:HE1  | 13       | 0.21          |
| (1,3047) | 1:57:A:PHE:HB3  | 1:42:A:TRP:HE1  | 37       | 0.21          |
| (1,3011) | 1:30:A:GLU:HB2  | 1:14:A:LYS:HE2  | 11       | 0.21          |
| (1,3004) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG21 | 15       | 0.21          |
| (1,3004) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG22 | 15       | 0.21          |
| (1,3004) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG23 | 15       | 0.21          |
| (1,3004) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG21 | 22       | 0.21          |
| (1,3004) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG22 | 22       | 0.21          |
| (1,3004) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG23 | 22       | 0.21          |
| (1,2996) | 1:15:A:ARG:HG2  | 1:93:A:SER:HB3  | 4        | 0.21          |
| (1,2968) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 8        | 0.21          |
| (1,2968) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 9        | 0.21          |
| (1,2968) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 16       | 0.21          |
| (1,2968) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 17       | 0.21          |
| (1,2968) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 19       | 0.21          |
| (1,2968) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 21       | 0.21          |
| (1,2968) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 22       | 0.21          |
| (1,2968) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 24       | 0.21          |
| (1,2968) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 28       | 0.21          |
| (1,2968) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 39       | 0.21          |
| (1,2968) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD3  | 40       | 0.21          |
| (1,2961) | 1:44:A:LYS:HE2  | 1:44:A:LYS:HG2  | 35       | 0.21          |
| (1,2931) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 17       | 0.21          |
| (1,2918) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 37       | 0.21          |
| (1,2879) | 1:102:A:ARG:HD3 | 1:102:A:ARG:HG2 | 3        | 0.21          |
| (1,2879) | 1:102:A:ARG:HD3 | 1:102:A:ARG:HG2 | 5        | 0.21          |
| (1,2879) | 1:102:A:ARG:HD3 | 1:102:A:ARG:HG2 | 8        | 0.21          |
| (1,2879) | 1:102:A:ARG:HD3 | 1:102:A:ARG:HG2 | 11       | 0.21          |
| (1,2879) | 1:102:A:ARG:HD3 | 1:102:A:ARG:HG2 | 23       | 0.21          |
| (1,2879) | 1:102:A:ARG:HD3 | 1:102:A:ARG:HG2 | 29       | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3  | 1:92:A:ARG:HG3  | 2        | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3  | 1:92:A:ARG:HG3  | 3        | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3  | 1:92:A:ARG:HG3  | 4        | 0.21          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,2857) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 5        | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 6        | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 7        | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 8        | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 11       | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 12       | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 15       | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 16       | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 17       | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 19       | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 20       | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 21       | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 22       | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 23       | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 24       | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 25       | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 26       | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 27       | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 28       | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 29       | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 30       | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 31       | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 32       | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 33       | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 34       | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 36       | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 37       | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 39       | 0.21          |
| (1,2857) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HG3 | 40       | 0.21          |
| (1,2802) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2 | 18       | 0.21          |
| (1,2802) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2 | 20       | 0.21          |
| (1,2802) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2 | 39       | 0.21          |
| (1,2801) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HG2 | 3        | 0.21          |
| (1,2801) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HG2 | 11       | 0.21          |
| (1,2801) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HG2 | 38       | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 1        | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 3        | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 4        | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 6        | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 7        | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 9        | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 10       | 0.21          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 12       | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 13       | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 14       | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 15       | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 16       | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 17       | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 18       | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 19       | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 20       | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 21       | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 22       | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 23       | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 24       | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 25       | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 26       | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 27       | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 28       | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 29       | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 32       | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 34       | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 35       | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 36       | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 37       | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 39       | 0.21          |
| (1,2796) | 1:15:A:ARG:HG3 | 1:15:A:ARG:HB3 | 40       | 0.21          |
| (1,2754) | 1:90:A:GLU:HB3 | 1:91:A:ALA:H   | 21       | 0.21          |
| (1,2754) | 1:90:A:GLU:HB3 | 1:91:A:ALA:H   | 28       | 0.21          |
| (1,2754) | 1:90:A:GLU:HB3 | 1:91:A:ALA:H   | 32       | 0.21          |
| (1,2754) | 1:90:A:GLU:HB3 | 1:91:A:ALA:H   | 40       | 0.21          |
| (1,2734) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 1        | 0.21          |
| (1,2734) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 4        | 0.21          |
| (1,2734) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 5        | 0.21          |
| (1,2734) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 8        | 0.21          |
| (1,2734) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 9        | 0.21          |
| (1,2734) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 12       | 0.21          |
| (1,2734) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 15       | 0.21          |
| (1,2734) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 16       | 0.21          |
| (1,2734) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 17       | 0.21          |
| (1,2734) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 19       | 0.21          |
| (1,2734) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 21       | 0.21          |
| (1,2734) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 22       | 0.21          |
| (1,2734) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 24       | 0.21          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,2734) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 27       | 0.21          |
| (1,2734) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 37       | 0.21          |
| (1,2718) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 1        | 0.21          |
| (1,2718) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 16       | 0.21          |
| (1,2718) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 19       | 0.21          |
| (1,2718) | 1:48:A:GLU:HG2 | 1:48:A:GLU:HA  | 33       | 0.21          |
| (1,2675) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 7        | 0.21          |
| (1,2668) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 4        | 0.21          |
| (1,2668) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 6        | 0.21          |
| (1,2668) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 7        | 0.21          |
| (1,2668) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 13       | 0.21          |
| (1,2668) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 26       | 0.21          |
| (1,2668) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 29       | 0.21          |
| (1,2668) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 33       | 0.21          |
| (1,2668) | 1:25:A:GLN:HG3 | 1:25:A:GLN:HA  | 38       | 0.21          |
| (1,2649) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H   | 5        | 0.21          |
| (1,2649) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H   | 26       | 0.21          |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 1        | 0.21          |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 4        | 0.21          |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 5        | 0.21          |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 7        | 0.21          |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 9        | 0.21          |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 10       | 0.21          |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 11       | 0.21          |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 12       | 0.21          |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 14       | 0.21          |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 15       | 0.21          |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 16       | 0.21          |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 17       | 0.21          |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 19       | 0.21          |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 20       | 0.21          |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 21       | 0.21          |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 22       | 0.21          |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 23       | 0.21          |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 24       | 0.21          |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 25       | 0.21          |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 29       | 0.21          |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 30       | 0.21          |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 32       | 0.21          |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 34       | 0.21          |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 35       | 0.21          |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 36       | 0.21          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 37       | 0.21          |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 38       | 0.21          |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 39       | 0.21          |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 40       | 0.21          |
| (1,2598) | 1:36:A:ASP:HB2 | 1:37:A:ASP:H   | 18       | 0.21          |
| (1,2598) | 1:36:A:ASP:HB2 | 1:37:A:ASP:H   | 29       | 0.21          |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 16       | 0.21          |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 17       | 0.21          |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 23       | 0.21          |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 25       | 0.21          |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 26       | 0.21          |
| (1,2550) | 1:92:A:ARG:HA  | 1:83:A:ALA:H   | 34       | 0.21          |
| (1,2550) | 1:92:A:ARG:HA  | 1:83:A:ALA:H   | 38       | 0.21          |
| (1,2534) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 2        | 0.21          |
| (1,2534) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 3        | 0.21          |
| (1,2534) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 6        | 0.21          |
| (1,2534) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 9        | 0.21          |
| (1,2534) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 17       | 0.21          |
| (1,2511) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 10       | 0.21          |
| (1,2485) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 22       | 0.21          |
| (1,2485) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 24       | 0.21          |
| (1,2485) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 25       | 0.21          |
| (1,2485) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 26       | 0.21          |
| (1,2485) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 27       | 0.21          |
| (1,2485) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 30       | 0.21          |
| (1,2485) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 32       | 0.21          |
| (1,2485) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 37       | 0.21          |
| (1,2485) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 38       | 0.21          |
| (1,2431) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 5        | 0.21          |
| (1,2431) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 14       | 0.21          |
| (1,2402) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 5        | 0.21          |
| (1,2402) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 5        | 0.21          |
| (1,2402) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 5        | 0.21          |
| (1,2402) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 14       | 0.21          |
| (1,2402) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 14       | 0.21          |
| (1,2402) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 14       | 0.21          |
| (1,2402) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 30       | 0.21          |
| (1,2402) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 30       | 0.21          |
| (1,2402) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 30       | 0.21          |
| (1,2322) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 2        | 0.21          |
| (1,2322) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 8        | 0.21          |
| (1,2322) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 12       | 0.21          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2322) | 1:80:A:SER:HB2  | 1:81:A:VAL:H   | 19       | 0.21          |
| (1,2322) | 1:80:A:SER:HB2  | 1:81:A:VAL:H   | 33       | 0.21          |
| (1,2322) | 1:80:A:SER:HB2  | 1:81:A:VAL:H   | 35       | 0.21          |
| (1,2286) | 1:96:A:GLU:HG2  | 1:97:A:LEU:H   | 20       | 0.21          |
| (1,2286) | 1:96:A:GLU:HG2  | 1:97:A:LEU:H   | 21       | 0.21          |
| (1,2286) | 1:96:A:GLU:HG2  | 1:97:A:LEU:H   | 29       | 0.21          |
| (1,2286) | 1:96:A:GLU:HG2  | 1:97:A:LEU:H   | 31       | 0.21          |
| (1,2286) | 1:96:A:GLU:HG2  | 1:97:A:LEU:H   | 33       | 0.21          |
| (1,2286) | 1:96:A:GLU:HG2  | 1:97:A:LEU:H   | 35       | 0.21          |
| (1,2286) | 1:96:A:GLU:HG2  | 1:97:A:LEU:H   | 39       | 0.21          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1 | 5        | 0.21          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2 | 5        | 0.21          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1 | 13       | 0.21          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2 | 13       | 0.21          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1 | 17       | 0.21          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2 | 17       | 0.21          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1 | 21       | 0.21          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2 | 21       | 0.21          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1 | 33       | 0.21          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2 | 33       | 0.21          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1 | 35       | 0.21          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2 | 35       | 0.21          |
| (1,2236) | 1:18:A:ASN:HB3  | 1:18:A:ASN:H   | 2        | 0.21          |
| (1,2236) | 1:18:A:ASN:HB3  | 1:18:A:ASN:H   | 14       | 0.21          |
| (1,2236) | 1:18:A:ASN:HB3  | 1:18:A:ASN:H   | 17       | 0.21          |
| (1,2236) | 1:18:A:ASN:HB3  | 1:18:A:ASN:H   | 18       | 0.21          |
| (1,2236) | 1:18:A:ASN:HB3  | 1:18:A:ASN:H   | 21       | 0.21          |
| (1,2236) | 1:18:A:ASN:HB3  | 1:18:A:ASN:H   | 30       | 0.21          |
| (1,2236) | 1:18:A:ASN:HB3  | 1:18:A:ASN:H   | 33       | 0.21          |
| (1,2236) | 1:18:A:ASN:HB3  | 1:18:A:ASN:H   | 34       | 0.21          |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H   | 3        | 0.21          |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H   | 14       | 0.21          |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H   | 15       | 0.21          |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H   | 26       | 0.21          |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H   | 29       | 0.21          |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H   | 34       | 0.21          |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H   | 40       | 0.21          |
| (1,2129) | 1:47:A:THR:HG21 | 1:47:A:THR:HB  | 5        | 0.21          |
| (1,2129) | 1:47:A:THR:HG22 | 1:47:A:THR:HB  | 5        | 0.21          |
| (1,2129) | 1:47:A:THR:HG23 | 1:47:A:THR:HB  | 5        | 0.21          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA  | 1        | 0.21          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA  | 1        | 0.21          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA  | 1        | 0.21          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 8        | 0.21          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 8        | 0.21          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 8        | 0.21          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 8        | 0.21          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 8        | 0.21          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 8        | 0.21          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 9        | 0.21          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 9        | 0.21          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 9        | 0.21          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 9        | 0.21          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 9        | 0.21          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 9        | 0.21          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 13       | 0.21          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 13       | 0.21          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 13       | 0.21          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 13       | 0.21          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 13       | 0.21          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 13       | 0.21          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 3        | 0.21          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 3        | 0.21          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 3        | 0.21          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 6        | 0.21          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 6        | 0.21          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 6        | 0.21          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 10       | 0.21          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 10       | 0.21          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 10       | 0.21          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 27       | 0.21          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 27       | 0.21          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 27       | 0.21          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 33       | 0.21          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 33       | 0.21          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 33       | 0.21          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 6        | 0.21          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 6        | 0.21          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 6        | 0.21          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 9        | 0.21          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 9        | 0.21          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 9        | 0.21          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 10       | 0.21          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 10       | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3  | 10       | 0.21          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3  | 15       | 0.21          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3  | 15       | 0.21          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3  | 15       | 0.21          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3  | 16       | 0.21          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3  | 16       | 0.21          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3  | 16       | 0.21          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3  | 17       | 0.21          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3  | 17       | 0.21          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3  | 17       | 0.21          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3  | 20       | 0.21          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3  | 20       | 0.21          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3  | 20       | 0.21          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3  | 21       | 0.21          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3  | 21       | 0.21          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3  | 21       | 0.21          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3  | 24       | 0.21          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3  | 24       | 0.21          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3  | 24       | 0.21          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3  | 29       | 0.21          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3  | 29       | 0.21          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3  | 29       | 0.21          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3  | 33       | 0.21          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3  | 33       | 0.21          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3  | 33       | 0.21          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3  | 39       | 0.21          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3  | 39       | 0.21          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3  | 39       | 0.21          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 19       | 0.21          |
| (1,1935) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2  | 4        | 0.21          |
| (1,1935) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2  | 10       | 0.21          |
| (1,1935) | 1:14:A:LYS:HE2  | 1:14:A:LYS:HD2  | 15       | 0.21          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2  | 5        | 0.21          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2  | 9        | 0.21          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2  | 10       | 0.21          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2  | 11       | 0.21          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2  | 18       | 0.21          |
| (1,1916) | 1:14:A:LYS:HG3  | 1:14:A:LYS:HD2  | 22       | 0.21          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 6        | 0.21          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 6        | 0.21          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 6        | 0.21          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 6        | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 6        | 0.21          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 6        | 0.21          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 6        | 0.21          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 6        | 0.21          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 6        | 0.21          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 7        | 0.21          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 7        | 0.21          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 7        | 0.21          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 7        | 0.21          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 7        | 0.21          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 7        | 0.21          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 7        | 0.21          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 7        | 0.21          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 7        | 0.21          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 23       | 0.21          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 23       | 0.21          |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 23       | 0.21          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 23       | 0.21          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 23       | 0.21          |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 23       | 0.21          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 23       | 0.21          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 23       | 0.21          |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 23       | 0.21          |
| (1,1904) | 1:66:A:MET:HE1  | 1:43:A:TYR:H    | 2        | 0.21          |
| (1,1904) | 1:66:A:MET:HE2  | 1:43:A:TYR:H    | 2        | 0.21          |
| (1,1904) | 1:66:A:MET:HE3  | 1:43:A:TYR:H    | 2        | 0.21          |
| (1,1904) | 1:66:A:MET:HE1  | 1:43:A:TYR:H    | 6        | 0.21          |
| (1,1904) | 1:66:A:MET:HE2  | 1:43:A:TYR:H    | 6        | 0.21          |
| (1,1904) | 1:66:A:MET:HE3  | 1:43:A:TYR:H    | 6        | 0.21          |
| (1,1904) | 1:66:A:MET:HE1  | 1:43:A:TYR:H    | 7        | 0.21          |
| (1,1904) | 1:66:A:MET:HE2  | 1:43:A:TYR:H    | 7        | 0.21          |
| (1,1904) | 1:66:A:MET:HE3  | 1:43:A:TYR:H    | 7        | 0.21          |
| (1,1904) | 1:66:A:MET:HE1  | 1:43:A:TYR:H    | 40       | 0.21          |
| (1,1904) | 1:66:A:MET:HE2  | 1:43:A:TYR:H    | 40       | 0.21          |
| (1,1904) | 1:66:A:MET:HE3  | 1:43:A:TYR:H    | 40       | 0.21          |
| (1,1825) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 1        | 0.21          |
| (1,1825) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 5        | 0.21          |
| (1,1825) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 6        | 0.21          |
| (1,1825) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 7        | 0.21          |
| (1,1825) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 10       | 0.21          |
| (1,1825) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 21       | 0.21          |
| (1,1825) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 23       | 0.21          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1825) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA   | 24       | 0.21          |
| (1,1825) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA   | 25       | 0.21          |
| (1,1825) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA   | 26       | 0.21          |
| (1,1825) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA   | 30       | 0.21          |
| (1,1825) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA   | 32       | 0.21          |
| (1,1825) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA   | 33       | 0.21          |
| (1,1825) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA   | 34       | 0.21          |
| (1,1825) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA   | 35       | 0.21          |
| (1,1825) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA   | 36       | 0.21          |
| (1,1825) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA   | 39       | 0.21          |
| (1,1825) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA   | 40       | 0.21          |
| (1,1812) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA   | 1        | 0.21          |
| (1,1812) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA   | 5        | 0.21          |
| (1,1812) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA   | 6        | 0.21          |
| (1,1812) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA   | 7        | 0.21          |
| (1,1812) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA   | 10       | 0.21          |
| (1,1812) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA   | 21       | 0.21          |
| (1,1812) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA   | 23       | 0.21          |
| (1,1812) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA   | 24       | 0.21          |
| (1,1812) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA   | 25       | 0.21          |
| (1,1812) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA   | 26       | 0.21          |
| (1,1812) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA   | 30       | 0.21          |
| (1,1812) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA   | 32       | 0.21          |
| (1,1812) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA   | 33       | 0.21          |
| (1,1812) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA   | 34       | 0.21          |
| (1,1812) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA   | 35       | 0.21          |
| (1,1812) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA   | 36       | 0.21          |
| (1,1812) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA   | 39       | 0.21          |
| (1,1812) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA   | 40       | 0.21          |
| (1,1778) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H    | 25       | 0.21          |
| (1,1778) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H    | 27       | 0.21          |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2  | 1        | 0.21          |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2  | 4        | 0.21          |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2  | 8        | 0.21          |
| (1,1728) | 1:48:A:GLU:HB2 | 1:48:A:GLU:H    | 12       | 0.21          |
| (1,1728) | 1:48:A:GLU:HB2 | 1:48:A:GLU:H    | 18       | 0.21          |
| (1,1728) | 1:48:A:GLU:HB2 | 1:48:A:GLU:H    | 19       | 0.21          |
| (1,1728) | 1:48:A:GLU:HB2 | 1:48:A:GLU:H    | 29       | 0.21          |
| (1,1717) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG11 | 36       | 0.21          |
| (1,1717) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG12 | 36       | 0.21          |
| (1,1717) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG13 | 36       | 0.21          |
| (1,1717) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG11 | 36       | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG12 | 36       | 0.21          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 36       | 0.21          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 36       | 0.21          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 36       | 0.21          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 36       | 0.21          |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 14       | 0.21          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 14       | 0.21          |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 14       | 0.21          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 4        | 0.21          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 4        | 0.21          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 4        | 0.21          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 4        | 0.21          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 4        | 0.21          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 4        | 0.21          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 4        | 0.21          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 4        | 0.21          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 4        | 0.21          |
| (1,1624) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2  | 21       | 0.21          |
| (1,1624) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2  | 21       | 0.21          |
| (1,1624) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2  | 21       | 0.21          |
| (1,1624) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2  | 32       | 0.21          |
| (1,1624) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2  | 32       | 0.21          |
| (1,1624) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2  | 32       | 0.21          |
| (1,1624) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2  | 34       | 0.21          |
| (1,1624) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2  | 34       | 0.21          |
| (1,1624) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2  | 34       | 0.21          |
| (1,1624) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2  | 39       | 0.21          |
| (1,1624) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2  | 39       | 0.21          |
| (1,1624) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2  | 39       | 0.21          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 3        | 0.21          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 3        | 0.21          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 3        | 0.21          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 4        | 0.21          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 4        | 0.21          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 4        | 0.21          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 7        | 0.21          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 7        | 0.21          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 7        | 0.21          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 25       | 0.21          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 25       | 0.21          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 25       | 0.21          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 33       | 0.21          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 33       | 0.21          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 33       | 0.21          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2 | 37       | 0.21          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 37       | 0.21          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 37       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB  | 1        | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB  | 1        | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB  | 1        | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB  | 3        | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB  | 3        | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB  | 3        | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB  | 4        | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB  | 4        | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB  | 4        | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB  | 5        | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB  | 5        | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB  | 5        | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB  | 6        | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB  | 6        | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB  | 6        | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB  | 7        | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB  | 7        | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB  | 7        | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB  | 8        | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB  | 8        | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB  | 8        | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB  | 9        | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB  | 9        | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB  | 9        | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB  | 10       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB  | 10       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB  | 10       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB  | 12       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB  | 12       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB  | 12       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB  | 13       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB  | 13       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB  | 13       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB  | 14       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB  | 14       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB  | 14       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB  | 15       | 0.21          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 15       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 15       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 16       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 16       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 16       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 17       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 17       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 17       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 18       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 18       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 18       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 19       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 19       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 19       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 20       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 20       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 20       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 21       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 21       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 21       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 22       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 22       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 22       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 23       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 23       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 23       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 25       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 25       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 25       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 26       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 26       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 26       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 27       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 27       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 27       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 28       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 28       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 28       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 29       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 29       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 29       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 30       | 0.21          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 30       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 30       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 31       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 31       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 31       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 32       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 32       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 32       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 33       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 33       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 33       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 34       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 34       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 34       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 35       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 35       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 35       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 37       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 37       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 37       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 39       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 39       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 39       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD11 | 1:39:A:ILE:HB | 40       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD12 | 1:39:A:ILE:HB | 40       | 0.21          |
| (1,1580) | 1:39:A:ILE:HD13 | 1:39:A:ILE:HB | 40       | 0.21          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA | 4        | 0.21          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA | 4        | 0.21          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA | 4        | 0.21          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA | 6        | 0.21          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA | 6        | 0.21          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA | 6        | 0.21          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA | 29       | 0.21          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA | 29       | 0.21          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA | 29       | 0.21          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA | 37       | 0.21          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA | 37       | 0.21          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA | 37       | 0.21          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H  | 9        | 0.21          |
| (1,1482) | 1:81:A:VAL:HB   | 1:82:A:ILE:H  | 20       | 0.21          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H  | 6        | 0.21          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H  | 6        | 0.21          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 6        | 0.21          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 11       | 0.21          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 11       | 0.21          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 11       | 0.21          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 15       | 0.21          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 15       | 0.21          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 15       | 0.21          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 16       | 0.21          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 16       | 0.21          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 16       | 0.21          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 17       | 0.21          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 17       | 0.21          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 17       | 0.21          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 20       | 0.21          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 20       | 0.21          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 20       | 0.21          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 26       | 0.21          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 26       | 0.21          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 26       | 0.21          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 40       | 0.21          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 40       | 0.21          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 40       | 0.21          |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 17       | 0.21          |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 17       | 0.21          |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 17       | 0.21          |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 21       | 0.21          |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 21       | 0.21          |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 21       | 0.21          |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 24       | 0.21          |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 24       | 0.21          |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 24       | 0.21          |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 34       | 0.21          |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 34       | 0.21          |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 34       | 0.21          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 9        | 0.21          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 9        | 0.21          |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 9        | 0.21          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 14       | 0.21          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 14       | 0.21          |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 14       | 0.21          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 15       | 0.21          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 15       | 0.21          |

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| Key      | Atom-1          | Atom-2       | Model ID | Violation (Å) |
|----------|-----------------|--------------|----------|---------------|
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H | 15       | 0.21          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H | 22       | 0.21          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H | 22       | 0.21          |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H | 22       | 0.21          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 3        | 0.21          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 3        | 0.21          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 3        | 0.21          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 19       | 0.21          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 19       | 0.21          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 19       | 0.21          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 36       | 0.21          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 36       | 0.21          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 36       | 0.21          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 40       | 0.21          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 40       | 0.21          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 40       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 2        | 0.21          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 2        | 0.21          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 2        | 0.21          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 4        | 0.21          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 4        | 0.21          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 4        | 0.21          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 5        | 0.21          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 5        | 0.21          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 5        | 0.21          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 7        | 0.21          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 7        | 0.21          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 7        | 0.21          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 8        | 0.21          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 8        | 0.21          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 8        | 0.21          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 10       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 10       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 10       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 13       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 13       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 13       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 14       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 14       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 14       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 15       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 15       | 0.21          |

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| Key      | Atom-1          | Atom-2       | Model ID | Violation (Å) |
|----------|-----------------|--------------|----------|---------------|
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 15       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 17       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 17       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 17       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 21       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 21       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 21       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 22       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 22       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 22       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 24       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 24       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 24       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 25       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 25       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 25       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 26       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 26       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 26       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 28       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 28       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 28       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 30       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 30       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 30       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 31       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 31       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 31       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 32       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 32       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 32       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 34       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 34       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 34       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 36       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 36       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 36       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 37       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 37       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 37       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 38       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 38       | 0.21          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H   | 38       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H   | 39       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H   | 39       | 0.21          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H   | 39       | 0.21          |
| (1,1396) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 4        | 0.21          |
| (1,1396) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 4        | 0.21          |
| (1,1396) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 4        | 0.21          |
| (1,1396) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 6        | 0.21          |
| (1,1396) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 6        | 0.21          |
| (1,1396) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 6        | 0.21          |
| (1,1396) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 9        | 0.21          |
| (1,1396) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 9        | 0.21          |
| (1,1396) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 9        | 0.21          |
| (1,1396) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 12       | 0.21          |
| (1,1396) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 12       | 0.21          |
| (1,1396) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 12       | 0.21          |
| (1,1396) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 17       | 0.21          |
| (1,1396) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 17       | 0.21          |
| (1,1396) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 17       | 0.21          |
| (1,1396) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 19       | 0.21          |
| (1,1396) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 19       | 0.21          |
| (1,1396) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 19       | 0.21          |
| (1,1396) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 20       | 0.21          |
| (1,1396) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 20       | 0.21          |
| (1,1396) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 20       | 0.21          |
| (1,1396) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 38       | 0.21          |
| (1,1396) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 38       | 0.21          |
| (1,1396) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 38       | 0.21          |
| (1,1396) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 40       | 0.21          |
| (1,1396) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 40       | 0.21          |
| (1,1396) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 40       | 0.21          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3 | 18       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 1        | 0.21          |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 1        | 0.21          |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 1        | 0.21          |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 3        | 0.21          |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 3        | 0.21          |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 3        | 0.21          |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 11       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 11       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 11       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 14       | 0.21          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 14       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 14       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 15       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 15       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 15       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 17       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 17       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 17       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 19       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 19       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 19       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 22       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 22       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 22       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 23       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 23       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 23       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 25       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 25       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 25       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 33       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 33       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 33       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 34       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 34       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 34       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 35       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 35       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 35       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 36       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 36       | 0.21          |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 36       | 0.21          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 3        | 0.21          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 3        | 0.21          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 3        | 0.21          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 7        | 0.21          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 7        | 0.21          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 7        | 0.21          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 17       | 0.21          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 17       | 0.21          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 17       | 0.21          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 18       | 0.21          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 18       | 0.21          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 18       | 0.21          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 19       | 0.21          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 19       | 0.21          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 19       | 0.21          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 25       | 0.21          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 25       | 0.21          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 25       | 0.21          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 30       | 0.21          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 30       | 0.21          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 30       | 0.21          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 38       | 0.21          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 38       | 0.21          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 38       | 0.21          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 1        | 0.21          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 9        | 0.21          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 13       | 0.21          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 16       | 0.21          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 20       | 0.21          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 21       | 0.21          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 22       | 0.21          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 26       | 0.21          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 30       | 0.21          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 35       | 0.21          |
| (1,1331) | 1:19:A:ILE:HG12 | 1:19:A:ILE:HB  | 38       | 0.21          |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA  | 3        | 0.21          |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA  | 3        | 0.21          |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA  | 3        | 0.21          |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA  | 7        | 0.21          |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA  | 7        | 0.21          |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA  | 7        | 0.21          |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA  | 10       | 0.21          |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA  | 10       | 0.21          |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA  | 10       | 0.21          |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA  | 11       | 0.21          |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA  | 11       | 0.21          |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA  | 11       | 0.21          |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA  | 14       | 0.21          |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA  | 14       | 0.21          |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA  | 14       | 0.21          |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA  | 19       | 0.21          |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA  | 19       | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 19       | 0.21          |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 20       | 0.21          |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 20       | 0.21          |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 20       | 0.21          |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 26       | 0.21          |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 26       | 0.21          |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 26       | 0.21          |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 27       | 0.21          |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 27       | 0.21          |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 27       | 0.21          |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 40       | 0.21          |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 40       | 0.21          |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 40       | 0.21          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 24       | 0.21          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 24       | 0.21          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 24       | 0.21          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 24       | 0.21          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 24       | 0.21          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 24       | 0.21          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 8        | 0.21          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 8        | 0.21          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 8        | 0.21          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 9        | 0.21          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 9        | 0.21          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 9        | 0.21          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 27       | 0.21          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 27       | 0.21          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 27       | 0.21          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 8        | 0.21          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 8        | 0.21          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 8        | 0.21          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 9        | 0.21          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 9        | 0.21          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 9        | 0.21          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 27       | 0.21          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 27       | 0.21          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 27       | 0.21          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 4        | 0.21          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 4        | 0.21          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 4        | 0.21          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 27       | 0.21          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 27       | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 27       | 0.21          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 28       | 0.21          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 28       | 0.21          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 28       | 0.21          |
| (1,1237) | 1:13:A:THR:HG21 | 1:34:A:SER:HB2  | 9        | 0.21          |
| (1,1237) | 1:13:A:THR:HG22 | 1:34:A:SER:HB2  | 9        | 0.21          |
| (1,1237) | 1:13:A:THR:HG23 | 1:34:A:SER:HB2  | 9        | 0.21          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 2        | 0.21          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 5        | 0.21          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 8        | 0.21          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 13       | 0.21          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 15       | 0.21          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 17       | 0.21          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 18       | 0.21          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 21       | 0.21          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 25       | 0.21          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 27       | 0.21          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 28       | 0.21          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 30       | 0.21          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 31       | 0.21          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 32       | 0.21          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 33       | 0.21          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 34       | 0.21          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 35       | 0.21          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 36       | 0.21          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 37       | 0.21          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 38       | 0.21          |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 16       | 0.21          |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 18       | 0.21          |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 19       | 0.21          |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 22       | 0.21          |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 23       | 0.21          |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 37       | 0.21          |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 38       | 0.21          |
| (1,1176) | 1:47:A:THR:H    | 1:44:A:LYS:HB3  | 5        | 0.21          |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 3        | 0.21          |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 6        | 0.21          |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 12       | 0.21          |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 14       | 0.21          |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 15       | 0.21          |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 18       | 0.21          |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 21       | 0.21          |

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| Key      | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|----------|---------------|----------------|----------|---------------|
| (1,1169) | 1:14:A:LYS:H  | 1:14:A:LYS:HD2 | 33       | 0.21          |
| (1,1169) | 1:14:A:LYS:H  | 1:14:A:LYS:HD2 | 38       | 0.21          |
| (1,1163) | 1:75:A:ASP:H  | 1:74:A:ASP:HB2 | 9        | 0.21          |
| (1,1163) | 1:75:A:ASP:H  | 1:74:A:ASP:HB2 | 13       | 0.21          |
| (1,1163) | 1:75:A:ASP:H  | 1:74:A:ASP:HB2 | 19       | 0.21          |
| (1,1163) | 1:75:A:ASP:H  | 1:74:A:ASP:HB2 | 30       | 0.21          |
| (1,1163) | 1:75:A:ASP:H  | 1:74:A:ASP:HB2 | 32       | 0.21          |
| (1,1163) | 1:75:A:ASP:H  | 1:74:A:ASP:HB2 | 34       | 0.21          |
| (1,1163) | 1:75:A:ASP:H  | 1:74:A:ASP:HB2 | 38       | 0.21          |
| (1,1163) | 1:75:A:ASP:H  | 1:74:A:ASP:HB2 | 39       | 0.21          |
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 19       | 0.21          |
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 21       | 0.21          |
| (1,1002) | 1:5:A:PHE:H   | 1:4:A:PRO:HA   | 20       | 0.21          |
| (1,969)  | 1:21:A:VAL:H  | 1:20:A:VAL:HB  | 4        | 0.21          |
| (1,969)  | 1:21:A:VAL:H  | 1:20:A:VAL:HB  | 11       | 0.21          |
| (1,969)  | 1:21:A:VAL:H  | 1:20:A:VAL:HB  | 12       | 0.21          |
| (1,969)  | 1:21:A:VAL:H  | 1:20:A:VAL:HB  | 21       | 0.21          |
| (1,969)  | 1:21:A:VAL:H  | 1:20:A:VAL:HB  | 24       | 0.21          |
| (1,969)  | 1:21:A:VAL:H  | 1:20:A:VAL:HB  | 25       | 0.21          |
| (1,969)  | 1:21:A:VAL:H  | 1:20:A:VAL:HB  | 30       | 0.21          |
| (1,969)  | 1:21:A:VAL:H  | 1:20:A:VAL:HB  | 31       | 0.21          |
| (1,969)  | 1:21:A:VAL:H  | 1:20:A:VAL:HB  | 37       | 0.21          |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB  | 9        | 0.21          |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB  | 15       | 0.21          |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB  | 34       | 0.21          |
| (1,919)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB2 | 18       | 0.21          |
| (1,919)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB2 | 29       | 0.21          |
| (1,918)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB3 | 16       | 0.21          |
| (1,918)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB3 | 17       | 0.21          |
| (1,918)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB3 | 23       | 0.21          |
| (1,918)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB3 | 25       | 0.21          |
| (1,918)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB3 | 26       | 0.21          |
| (1,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3  | 32       | 0.21          |
| (1,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3  | 35       | 0.21          |
| (1,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3  | 37       | 0.21          |
| (1,870)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD2  | 4        | 0.21          |
| (1,870)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD2  | 6        | 0.21          |
| (1,870)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD2  | 14       | 0.21          |
| (1,870)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD2  | 18       | 0.21          |
| (1,870)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD2  | 20       | 0.21          |
| (1,870)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD2  | 30       | 0.21          |
| (1,869)  | 1:8:A:GLU:H   | 1:7:A:ALA:HA   | 20       | 0.21          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,849) | 1:83:A:ALA:H  | 1:91:A:ALA:HB1  | 7        | 0.21          |
| (1,849) | 1:83:A:ALA:H  | 1:91:A:ALA:HB2  | 7        | 0.21          |
| (1,849) | 1:83:A:ALA:H  | 1:91:A:ALA:HB3  | 7        | 0.21          |
| (1,849) | 1:83:A:ALA:H  | 1:91:A:ALA:HB1  | 12       | 0.21          |
| (1,849) | 1:83:A:ALA:H  | 1:91:A:ALA:HB2  | 12       | 0.21          |
| (1,849) | 1:83:A:ALA:H  | 1:91:A:ALA:HB3  | 12       | 0.21          |
| (1,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG21 | 3        | 0.21          |
| (1,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG22 | 3        | 0.21          |
| (1,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG23 | 3        | 0.21          |
| (1,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG21 | 9        | 0.21          |
| (1,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG22 | 9        | 0.21          |
| (1,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG23 | 9        | 0.21          |
| (1,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG21 | 14       | 0.21          |
| (1,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG22 | 14       | 0.21          |
| (1,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG23 | 14       | 0.21          |
| (1,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG21 | 24       | 0.21          |
| (1,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG22 | 24       | 0.21          |
| (1,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG23 | 24       | 0.21          |
| (1,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG21 | 32       | 0.21          |
| (1,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG22 | 32       | 0.21          |
| (1,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG23 | 32       | 0.21          |
| (1,801) | 1:54:A:LYS:H  | 1:54:A:LYS:HD2  | 17       | 0.21          |
| (1,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 4        | 0.21          |
| (1,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 13       | 0.21          |
| (1,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 15       | 0.21          |
| (1,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 16       | 0.21          |
| (1,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 18       | 0.21          |
| (1,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 20       | 0.21          |
| (1,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 25       | 0.21          |
| (1,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 28       | 0.21          |
| (1,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 30       | 0.21          |
| (1,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 31       | 0.21          |
| (1,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 34       | 0.21          |
| (1,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 37       | 0.21          |
| (1,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 38       | 0.21          |
| (1,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 39       | 0.21          |
| (1,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 8        | 0.21          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 10       | 0.21          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 11       | 0.21          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 19       | 0.21          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 27       | 0.21          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 28       | 0.21          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3 | 39       | 0.21          |
| (1,590) | 1:3:A:ASP:H   | 1:2:A:ILE:HA   | 10       | 0.21          |
| (1,590) | 1:3:A:ASP:H   | 1:2:A:ILE:HA   | 12       | 0.21          |
| (1,590) | 1:3:A:ASP:H   | 1:2:A:ILE:HA   | 14       | 0.21          |
| (1,590) | 1:3:A:ASP:H   | 1:2:A:ILE:HA   | 17       | 0.21          |
| (1,590) | 1:3:A:ASP:H   | 1:2:A:ILE:HA   | 19       | 0.21          |
| (1,590) | 1:3:A:ASP:H   | 1:2:A:ILE:HA   | 28       | 0.21          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1 | 6        | 0.21          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2 | 6        | 0.21          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1 | 16       | 0.21          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2 | 16       | 0.21          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1 | 28       | 0.21          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2 | 28       | 0.21          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1 | 29       | 0.21          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2 | 29       | 0.21          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1 | 37       | 0.21          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2 | 37       | 0.21          |
| (1,556) | 1:47:A:THR:H  | 1:48:A:GLU:H   | 6        | 0.21          |
| (1,556) | 1:47:A:THR:H  | 1:48:A:GLU:H   | 8        | 0.21          |
| (1,556) | 1:47:A:THR:H  | 1:48:A:GLU:H   | 10       | 0.21          |
| (1,556) | 1:47:A:THR:H  | 1:48:A:GLU:H   | 19       | 0.21          |
| (1,556) | 1:47:A:THR:H  | 1:48:A:GLU:H   | 26       | 0.21          |
| (1,556) | 1:47:A:THR:H  | 1:48:A:GLU:H   | 28       | 0.21          |
| (1,556) | 1:47:A:THR:H  | 1:48:A:GLU:H   | 29       | 0.21          |
| (1,556) | 1:47:A:THR:H  | 1:48:A:GLU:H   | 37       | 0.21          |
| (1,556) | 1:47:A:THR:H  | 1:48:A:GLU:H   | 38       | 0.21          |
| (1,549) | 1:71:A:VAL:H  | 1:70:A:ASN:HB2 | 4        | 0.21          |
| (1,549) | 1:71:A:VAL:H  | 1:70:A:ASN:HB2 | 13       | 0.21          |
| (1,549) | 1:71:A:VAL:H  | 1:70:A:ASN:HB2 | 16       | 0.21          |
| (1,549) | 1:71:A:VAL:H  | 1:70:A:ASN:HB2 | 35       | 0.21          |
| (1,549) | 1:71:A:VAL:H  | 1:70:A:ASN:HB2 | 37       | 0.21          |
| (1,546) | 1:71:A:VAL:H  | 1:24:A:HIS:HA  | 31       | 0.21          |
| (1,529) | 1:99:A:GLY:H  | 1:76:A:GLU:HB2 | 34       | 0.21          |
| (1,525) | 1:99:A:GLY:H  | 1:100:A:GLU:H  | 9        | 0.21          |
| (1,525) | 1:99:A:GLY:H  | 1:100:A:GLU:H  | 34       | 0.21          |
| (1,513) | 1:67:A:THR:H  | 1:66:A:MET:HG3 | 21       | 0.21          |
| (1,513) | 1:67:A:THR:H  | 1:66:A:MET:HG3 | 24       | 0.21          |
| (1,513) | 1:67:A:THR:H  | 1:66:A:MET:HG3 | 33       | 0.21          |
| (1,423) | 1:69:A:HIS:H  | 1:69:A:HIS:HD2 | 2        | 0.21          |
| (1,423) | 1:69:A:HIS:H  | 1:69:A:HIS:HD2 | 3        | 0.21          |
| (1,423) | 1:69:A:HIS:H  | 1:69:A:HIS:HD2 | 19       | 0.21          |
| (1,423) | 1:69:A:HIS:H  | 1:69:A:HIS:HD2 | 20       | 0.21          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,423) | 1:69:A:HIS:H  | 1:69:A:HIS:HD2  | 36       | 0.21          |
| (1,423) | 1:69:A:HIS:H  | 1:69:A:HIS:HD2  | 37       | 0.21          |
| (1,416) | 1:96:A:GLU:H  | 1:96:A:GLU:HB3  | 28       | 0.21          |
| (1,394) | 1:77:A:GLY:H  | 1:97:A:LEU:HA   | 21       | 0.21          |
| (1,394) | 1:77:A:GLY:H  | 1:97:A:LEU:HA   | 31       | 0.21          |
| (1,394) | 1:77:A:GLY:H  | 1:97:A:LEU:HA   | 39       | 0.21          |
| (1,369) | 1:18:A:ASN:H  | 1:17:A:GLN:HB2  | 5        | 0.21          |
| (1,369) | 1:18:A:ASN:H  | 1:17:A:GLN:HB2  | 26       | 0.21          |
| (1,366) | 1:18:A:ASN:H  | 1:18:A:ASN:HB3  | 2        | 0.21          |
| (1,366) | 1:18:A:ASN:H  | 1:18:A:ASN:HB3  | 14       | 0.21          |
| (1,366) | 1:18:A:ASN:H  | 1:18:A:ASN:HB3  | 17       | 0.21          |
| (1,366) | 1:18:A:ASN:H  | 1:18:A:ASN:HB3  | 18       | 0.21          |
| (1,366) | 1:18:A:ASN:H  | 1:18:A:ASN:HB3  | 21       | 0.21          |
| (1,366) | 1:18:A:ASN:H  | 1:18:A:ASN:HB3  | 30       | 0.21          |
| (1,366) | 1:18:A:ASN:H  | 1:18:A:ASN:HB3  | 33       | 0.21          |
| (1,366) | 1:18:A:ASN:H  | 1:18:A:ASN:HB3  | 34       | 0.21          |
| (1,343) | 1:14:A:LYS:H  | 1:33:A:VAL:HA   | 4        | 0.21          |
| (1,343) | 1:14:A:LYS:H  | 1:33:A:VAL:HA   | 11       | 0.21          |
| (1,343) | 1:14:A:LYS:H  | 1:33:A:VAL:HA   | 19       | 0.21          |
| (1,343) | 1:14:A:LYS:H  | 1:33:A:VAL:HA   | 25       | 0.21          |
| (1,343) | 1:14:A:LYS:H  | 1:33:A:VAL:HA   | 26       | 0.21          |
| (1,343) | 1:14:A:LYS:H  | 1:33:A:VAL:HA   | 39       | 0.21          |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 8        | 0.21          |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 8        | 0.21          |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 8        | 0.21          |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 9        | 0.21          |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 9        | 0.21          |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 9        | 0.21          |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 27       | 0.21          |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 27       | 0.21          |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 27       | 0.21          |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG21 | 10       | 0.21          |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG22 | 10       | 0.21          |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG23 | 10       | 0.21          |
| (1,176) | 1:10:A:ILE:H  | 1:35:A:PHE:HD1  | 23       | 0.21          |
| (1,176) | 1:10:A:ILE:H  | 1:35:A:PHE:HD2  | 23       | 0.21          |
| (1,148) | 1:45:A:GLY:H  | 1:46:A:PRO:HD2  | 11       | 0.21          |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 19       | 0.21          |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 21       | 0.21          |
| (1,133) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 10       | 0.21          |
| (1,133) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 12       | 0.21          |
| (1,133) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 35       | 0.21          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,133)  | 1:39:A:ILE:H   | 1:39:A:ILE:HG13 | 40       | 0.21          |
| (1,100)  | 1:22:A:SER:H   | 1:21:A:VAL:HB   | 8        | 0.21          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 1        | 0.21          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 1        | 0.21          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 1        | 0.21          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 2        | 0.21          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 2        | 0.21          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 2        | 0.21          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 5        | 0.21          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 5        | 0.21          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 5        | 0.21          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 9        | 0.21          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 9        | 0.21          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 9        | 0.21          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 15       | 0.21          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 15       | 0.21          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 15       | 0.21          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 17       | 0.21          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 17       | 0.21          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 17       | 0.21          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 26       | 0.21          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 26       | 0.21          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 26       | 0.21          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 28       | 0.21          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 28       | 0.21          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 28       | 0.21          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 29       | 0.21          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 29       | 0.21          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 29       | 0.21          |
| (1,22)   | 1:89:A:GLY:H   | 1:85:A:LEU:H    | 5        | 0.21          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 32       | 0.2           |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 32       | 0.2           |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 35       | 0.2           |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 35       | 0.2           |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 3        | 0.2           |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 3        | 0.2           |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 3        | 0.2           |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 3        | 0.2           |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 3        | 0.2           |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 3        | 0.2           |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 29       | 0.2           |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 29       | 0.2           |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 29       | 0.2           |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 29       | 0.2           |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 29       | 0.2           |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 29       | 0.2           |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 7        | 0.2           |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 7        | 0.2           |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 7        | 0.2           |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 7        | 0.2           |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 4        | 0.2           |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 7        | 0.2           |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 8        | 0.2           |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 26       | 0.2           |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 31       | 0.2           |
| (3,3143) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3  | 34       | 0.2           |
| (3,3143) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 34       | 0.2           |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2  | 35       | 0.2           |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2  | 35       | 0.2           |
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 23       | 0.2           |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 23       | 0.2           |
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 33       | 0.2           |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 33       | 0.2           |
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 34       | 0.2           |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 34       | 0.2           |
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 36       | 0.2           |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 36       | 0.2           |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 20       | 0.2           |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 23       | 0.2           |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 25       | 0.2           |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 34       | 0.2           |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 2        | 0.2           |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 2        | 0.2           |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 2        | 0.2           |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 3        | 0.2           |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 3        | 0.2           |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 3        | 0.2           |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 11       | 0.2           |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 11       | 0.2           |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 11       | 0.2           |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 24       | 0.2           |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 24       | 0.2           |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 24       | 0.2           |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 33       | 0.2           |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 33       | 0.2           |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 33       | 0.2           |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 35       | 0.2           |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 35       | 0.2           |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 35       | 0.2           |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 36       | 0.2           |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 36       | 0.2           |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 36       | 0.2           |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 37       | 0.2           |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 37       | 0.2           |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 37       | 0.2           |
| (3,3004) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 17       | 0.2           |
| (3,3004) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 26       | 0.2           |
| (3,2977) | 1:53:A:GLN:HG3 | 1:53:A:GLN:HB2  | 35       | 0.2           |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1  | 34       | 0.2           |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2  | 34       | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 1        | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 2        | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 3        | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 4        | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 5        | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 6        | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 7        | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 8        | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 9        | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 10       | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 11       | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 13       | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 14       | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 15       | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 16       | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 17       | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 18       | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 20       | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 22       | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 23       | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 24       | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 25       | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 26       | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 27       | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 28       | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 29       | 0.2           |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2874) | 1:92:A:ARG:HD2  | 1:92:A:ARG:HG2 | 30       | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2  | 1:92:A:ARG:HG2 | 31       | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2  | 1:92:A:ARG:HG2 | 33       | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2  | 1:92:A:ARG:HG2 | 34       | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2  | 1:92:A:ARG:HG2 | 35       | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2  | 1:92:A:ARG:HG2 | 36       | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2  | 1:92:A:ARG:HG2 | 37       | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2  | 1:92:A:ARG:HG2 | 38       | 0.2           |
| (3,2874) | 1:92:A:ARG:HD2  | 1:92:A:ARG:HG2 | 40       | 0.2           |
| (3,2809) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HB2 | 14       | 0.2           |
| (3,2809) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HB2 | 15       | 0.2           |
| (3,2809) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HB2 | 23       | 0.2           |
| (3,2809) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HB2 | 29       | 0.2           |
| (3,2809) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HB2 | 32       | 0.2           |
| (3,2809) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HB2 | 36       | 0.2           |
| (3,2809) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HB2 | 40       | 0.2           |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H  | 14       | 0.2           |
| (3,2761) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H   | 7        | 0.2           |
| (3,2761) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H   | 27       | 0.2           |
| (3,2761) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H   | 30       | 0.2           |
| (3,2748) | 1:86:A:GLU:HG3  | 1:87:A:PRO:HA  | 28       | 0.2           |
| (3,2738) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 2        | 0.2           |
| (3,2738) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 3        | 0.2           |
| (3,2738) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 6        | 0.2           |
| (3,2738) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 7        | 0.2           |
| (3,2738) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 10       | 0.2           |
| (3,2738) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 11       | 0.2           |
| (3,2738) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 13       | 0.2           |
| (3,2738) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 14       | 0.2           |
| (3,2738) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 18       | 0.2           |
| (3,2738) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 20       | 0.2           |
| (3,2738) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 23       | 0.2           |
| (3,2738) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 25       | 0.2           |
| (3,2738) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 26       | 0.2           |
| (3,2738) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 28       | 0.2           |
| (3,2738) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 29       | 0.2           |
| (3,2738) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 30       | 0.2           |
| (3,2738) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 31       | 0.2           |
| (3,2738) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 32       | 0.2           |
| (3,2738) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 33       | 0.2           |
| (3,2738) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 34       | 0.2           |
| (3,2738) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 35       | 0.2           |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,2738) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 36       | 0.2           |
| (3,2738) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 38       | 0.2           |
| (3,2738) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 39       | 0.2           |
| (3,2738) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 40       | 0.2           |
| (3,2689) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 16       | 0.2           |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 2        | 0.2           |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 3        | 0.2           |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 8        | 0.2           |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 13       | 0.2           |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 18       | 0.2           |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 26       | 0.2           |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 27       | 0.2           |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 28       | 0.2           |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 31       | 0.2           |
| (3,2630) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 33       | 0.2           |
| (3,2617) | 1:74:A:ASP:HB2 | 1:74:A:ASP:HA  | 17       | 0.2           |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 8        | 0.2           |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 11       | 0.2           |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 13       | 0.2           |
| (3,2538) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 1        | 0.2           |
| (3,2538) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 19       | 0.2           |
| (3,2538) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 20       | 0.2           |
| (3,2514) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 9        | 0.2           |
| (3,2514) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 12       | 0.2           |
| (3,2514) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 19       | 0.2           |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 23       | 0.2           |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 29       | 0.2           |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 31       | 0.2           |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 33       | 0.2           |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 34       | 0.2           |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 36       | 0.2           |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 39       | 0.2           |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 40       | 0.2           |
| (3,2434) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 23       | 0.2           |
| (3,2434) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 28       | 0.2           |
| (3,2434) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 29       | 0.2           |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 17       | 0.2           |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 17       | 0.2           |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 17       | 0.2           |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 5        | 0.2           |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 6        | 0.2           |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 7        | 0.2           |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 9        | 0.2           |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 34       | 0.2           |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 3        | 0.2           |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 7        | 0.2           |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 11       | 0.2           |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 13       | 0.2           |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 26       | 0.2           |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 2        | 0.2           |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 9        | 0.2           |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 10       | 0.2           |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 11       | 0.2           |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 13       | 0.2           |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 17       | 0.2           |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 22       | 0.2           |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 24       | 0.2           |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 25       | 0.2           |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 30       | 0.2           |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 32       | 0.2           |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 34       | 0.2           |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 36       | 0.2           |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 38       | 0.2           |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 12       | 0.2           |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1 | 7        | 0.2           |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2 | 7        | 0.2           |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1 | 12       | 0.2           |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2 | 12       | 0.2           |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1 | 20       | 0.2           |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2 | 20       | 0.2           |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1 | 22       | 0.2           |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2 | 22       | 0.2           |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1 | 24       | 0.2           |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2 | 24       | 0.2           |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1 | 30       | 0.2           |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2 | 30       | 0.2           |
| (3,2239) | 1:18:A:ASN:HB3 | 1:18:A:ASN:H   | 4        | 0.2           |
| (3,2239) | 1:18:A:ASN:HB3 | 1:18:A:ASN:H   | 11       | 0.2           |
| (3,2239) | 1:18:A:ASN:HB3 | 1:18:A:ASN:H   | 13       | 0.2           |
| (3,2239) | 1:18:A:ASN:HB3 | 1:18:A:ASN:H   | 24       | 0.2           |
| (3,2239) | 1:18:A:ASN:HB3 | 1:18:A:ASN:H   | 25       | 0.2           |
| (3,2239) | 1:18:A:ASN:HB3 | 1:18:A:ASN:H   | 32       | 0.2           |
| (3,2239) | 1:18:A:ASN:HB3 | 1:18:A:ASN:H   | 35       | 0.2           |
| (3,2239) | 1:18:A:ASN:HB3 | 1:18:A:ASN:H   | 36       | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2239) | 1:18:A:ASN:HB3  | 1:18:A:ASN:H    | 38       | 0.2           |
| (3,2239) | 1:18:A:ASN:HB3  | 1:18:A:ASN:H    | 39       | 0.2           |
| (3,2239) | 1:18:A:ASN:HB3  | 1:18:A:ASN:H    | 40       | 0.2           |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 5        | 0.2           |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 7        | 0.2           |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 9        | 0.2           |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 10       | 0.2           |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 25       | 0.2           |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 28       | 0.2           |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 32       | 0.2           |
| (3,2146) | 1:94:A:THR:HB   | 1:78:A:VAL:HG11 | 28       | 0.2           |
| (3,2146) | 1:94:A:THR:HB   | 1:78:A:VAL:HG12 | 28       | 0.2           |
| (3,2146) | 1:94:A:THR:HB   | 1:78:A:VAL:HG13 | 28       | 0.2           |
| (3,2102) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HA   | 36       | 0.2           |
| (3,2102) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HA   | 36       | 0.2           |
| (3,2102) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HA   | 36       | 0.2           |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 31       | 0.2           |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 31       | 0.2           |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 31       | 0.2           |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD11 | 5        | 0.2           |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD12 | 5        | 0.2           |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD13 | 5        | 0.2           |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD11 | 5        | 0.2           |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD12 | 5        | 0.2           |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD13 | 5        | 0.2           |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD11 | 5        | 0.2           |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD12 | 5        | 0.2           |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD13 | 5        | 0.2           |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD11 | 14       | 0.2           |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD12 | 14       | 0.2           |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD13 | 14       | 0.2           |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD11 | 14       | 0.2           |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD12 | 14       | 0.2           |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD13 | 14       | 0.2           |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD11 | 14       | 0.2           |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD12 | 14       | 0.2           |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD13 | 14       | 0.2           |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1  | 35       | 0.2           |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2  | 35       | 0.2           |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1  | 35       | 0.2           |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2  | 35       | 0.2           |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1  | 35       | 0.2           |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 35       | 0.2           |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 8        | 0.2           |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 8        | 0.2           |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 8        | 0.2           |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 12       | 0.2           |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 12       | 0.2           |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 12       | 0.2           |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 2        | 0.2           |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 2        | 0.2           |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 2        | 0.2           |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 3        | 0.2           |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 3        | 0.2           |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 3        | 0.2           |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 4        | 0.2           |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 4        | 0.2           |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 4        | 0.2           |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 8        | 0.2           |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 8        | 0.2           |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 8        | 0.2           |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 14       | 0.2           |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 14       | 0.2           |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 14       | 0.2           |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 28       | 0.2           |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 28       | 0.2           |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 28       | 0.2           |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA  | 17       | 0.2           |
| (3,1907) | 1:66:A:MET:HE1  | 1:43:A:TYR:H   | 10       | 0.2           |
| (3,1907) | 1:66:A:MET:HE2  | 1:43:A:TYR:H   | 10       | 0.2           |
| (3,1907) | 1:66:A:MET:HE3  | 1:43:A:TYR:H   | 10       | 0.2           |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 8        | 0.2           |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 8        | 0.2           |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 8        | 0.2           |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 33       | 0.2           |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 33       | 0.2           |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 33       | 0.2           |
| (3,1828) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA  | 3        | 0.2           |
| (3,1828) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA  | 4        | 0.2           |
| (3,1828) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA  | 8        | 0.2           |
| (3,1828) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA  | 9        | 0.2           |
| (3,1828) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA  | 12       | 0.2           |
| (3,1828) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA  | 14       | 0.2           |
| (3,1828) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA  | 19       | 0.2           |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,1828) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 20       | 0.2           |
| (3,1828) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 28       | 0.2           |
| (3,1815) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 3        | 0.2           |
| (3,1815) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 4        | 0.2           |
| (3,1815) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 8        | 0.2           |
| (3,1815) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 9        | 0.2           |
| (3,1815) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 12       | 0.2           |
| (3,1815) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 14       | 0.2           |
| (3,1815) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 19       | 0.2           |
| (3,1815) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 20       | 0.2           |
| (3,1815) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 28       | 0.2           |
| (3,1781) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 39       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 2        | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 3        | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 5        | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 6        | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 7        | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 9        | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 10       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 11       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 12       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 13       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 14       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 15       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 16       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 17       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 18       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 19       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 20       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 21       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 22       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 23       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 24       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 25       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 26       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 27       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 28       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 29       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 30       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 31       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 32       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 33       | 0.2           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (3,1743) | 1:51:A:GLU:HG2   | 1:51:A:GLU:HB2  | 34       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2   | 1:51:A:GLU:HB2  | 35       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2   | 1:51:A:GLU:HB2  | 36       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2   | 1:51:A:GLU:HB2  | 37       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2   | 1:51:A:GLU:HB2  | 38       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2   | 1:51:A:GLU:HB2  | 39       | 0.2           |
| (3,1743) | 1:51:A:GLU:HG2   | 1:51:A:GLU:HB2  | 40       | 0.2           |
| (3,1731) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H    | 2        | 0.2           |
| (3,1731) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H    | 5        | 0.2           |
| (3,1731) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H    | 9        | 0.2           |
| (3,1731) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H    | 11       | 0.2           |
| (3,1731) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H    | 15       | 0.2           |
| (3,1731) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H    | 16       | 0.2           |
| (3,1731) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H    | 34       | 0.2           |
| (3,1731) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H    | 37       | 0.2           |
| (3,1731) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H    | 39       | 0.2           |
| (3,1721) | 1:38:A:ALA:HB1   | 1:33:A:VAL:HG11 | 11       | 0.2           |
| (3,1721) | 1:38:A:ALA:HB1   | 1:33:A:VAL:HG12 | 11       | 0.2           |
| (3,1721) | 1:38:A:ALA:HB1   | 1:33:A:VAL:HG13 | 11       | 0.2           |
| (3,1721) | 1:38:A:ALA:HB2   | 1:33:A:VAL:HG11 | 11       | 0.2           |
| (3,1721) | 1:38:A:ALA:HB2   | 1:33:A:VAL:HG12 | 11       | 0.2           |
| (3,1721) | 1:38:A:ALA:HB2   | 1:33:A:VAL:HG13 | 11       | 0.2           |
| (3,1721) | 1:38:A:ALA:HB3   | 1:33:A:VAL:HG11 | 11       | 0.2           |
| (3,1721) | 1:38:A:ALA:HB3   | 1:33:A:VAL:HG12 | 11       | 0.2           |
| (3,1721) | 1:38:A:ALA:HB3   | 1:33:A:VAL:HG13 | 11       | 0.2           |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 1        | 0.2           |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 1        | 0.2           |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 1        | 0.2           |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 2        | 0.2           |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 2        | 0.2           |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 2        | 0.2           |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 4        | 0.2           |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 4        | 0.2           |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 4        | 0.2           |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 6        | 0.2           |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 6        | 0.2           |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 6        | 0.2           |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 7        | 0.2           |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 7        | 0.2           |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 7        | 0.2           |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 17       | 0.2           |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 17       | 0.2           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 17       | 0.2           |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 18       | 0.2           |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 18       | 0.2           |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 18       | 0.2           |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 20       | 0.2           |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 20       | 0.2           |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 20       | 0.2           |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 22       | 0.2           |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 22       | 0.2           |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 22       | 0.2           |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 37       | 0.2           |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 37       | 0.2           |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 37       | 0.2           |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 39       | 0.2           |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 39       | 0.2           |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 39       | 0.2           |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 40       | 0.2           |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 40       | 0.2           |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 40       | 0.2           |
| (3,1682) | 1:85:A:LEU:HD11  | 1:85:A:LEU:HA   | 18       | 0.2           |
| (3,1682) | 1:85:A:LEU:HD12  | 1:85:A:LEU:HA   | 18       | 0.2           |
| (3,1682) | 1:85:A:LEU:HD13  | 1:85:A:LEU:HA   | 18       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG21  | 1:16:A:ILE:HG21 | 2        | 0.2           |
| (3,1643) | 1:81:A:VAL:HG21  | 1:16:A:ILE:HG22 | 2        | 0.2           |
| (3,1643) | 1:81:A:VAL:HG21  | 1:16:A:ILE:HG23 | 2        | 0.2           |
| (3,1643) | 1:81:A:VAL:HG22  | 1:16:A:ILE:HG21 | 2        | 0.2           |
| (3,1643) | 1:81:A:VAL:HG22  | 1:16:A:ILE:HG22 | 2        | 0.2           |
| (3,1643) | 1:81:A:VAL:HG22  | 1:16:A:ILE:HG23 | 2        | 0.2           |
| (3,1643) | 1:81:A:VAL:HG23  | 1:16:A:ILE:HG21 | 2        | 0.2           |
| (3,1643) | 1:81:A:VAL:HG23  | 1:16:A:ILE:HG22 | 2        | 0.2           |
| (3,1643) | 1:81:A:VAL:HG23  | 1:16:A:ILE:HG23 | 2        | 0.2           |
| (3,1643) | 1:81:A:VAL:HG21  | 1:16:A:ILE:HG21 | 3        | 0.2           |
| (3,1643) | 1:81:A:VAL:HG21  | 1:16:A:ILE:HG22 | 3        | 0.2           |
| (3,1643) | 1:81:A:VAL:HG21  | 1:16:A:ILE:HG23 | 3        | 0.2           |
| (3,1643) | 1:81:A:VAL:HG22  | 1:16:A:ILE:HG21 | 3        | 0.2           |
| (3,1643) | 1:81:A:VAL:HG22  | 1:16:A:ILE:HG22 | 3        | 0.2           |
| (3,1643) | 1:81:A:VAL:HG22  | 1:16:A:ILE:HG23 | 3        | 0.2           |
| (3,1643) | 1:81:A:VAL:HG23  | 1:16:A:ILE:HG21 | 3        | 0.2           |
| (3,1643) | 1:81:A:VAL:HG23  | 1:16:A:ILE:HG22 | 3        | 0.2           |
| (3,1643) | 1:81:A:VAL:HG23  | 1:16:A:ILE:HG23 | 3        | 0.2           |
| (3,1643) | 1:81:A:VAL:HG21  | 1:16:A:ILE:HG21 | 7        | 0.2           |
| (3,1643) | 1:81:A:VAL:HG21  | 1:16:A:ILE:HG22 | 7        | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 7        | 0.2           |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 7        | 0.2           |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 7        | 0.2           |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 7        | 0.2           |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 7        | 0.2           |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 7        | 0.2           |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 7        | 0.2           |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 24       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 24       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 24       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 24       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 24       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 24       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 24       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 24       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 24       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 26       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 26       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 26       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 26       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 26       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 26       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 26       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 26       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 26       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 27       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 27       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 27       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 27       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 27       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 27       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 27       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 27       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 27       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 37       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 37       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 37       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 37       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 37       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 37       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 37       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 37       | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 37       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 38       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 38       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 38       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 38       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 38       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 38       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 38       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 38       | 0.2           |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 38       | 0.2           |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 9        | 0.2           |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 9        | 0.2           |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 9        | 0.2           |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 17       | 0.2           |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 17       | 0.2           |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 17       | 0.2           |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 20       | 0.2           |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 20       | 0.2           |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 20       | 0.2           |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 21       | 0.2           |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 21       | 0.2           |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 21       | 0.2           |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 30       | 0.2           |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 30       | 0.2           |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 30       | 0.2           |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 32       | 0.2           |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 32       | 0.2           |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 32       | 0.2           |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 32       | 0.2           |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 32       | 0.2           |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 32       | 0.2           |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 1        | 0.2           |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 1        | 0.2           |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 1        | 0.2           |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 12       | 0.2           |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 12       | 0.2           |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 12       | 0.2           |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 14       | 0.2           |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 14       | 0.2           |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 14       | 0.2           |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 15       | 0.2           |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 15       | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 15       | 0.2           |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 19       | 0.2           |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 19       | 0.2           |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 19       | 0.2           |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 27       | 0.2           |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 27       | 0.2           |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 27       | 0.2           |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 28       | 0.2           |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 28       | 0.2           |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 28       | 0.2           |
| (3,1539) | 1:2:A:ILE:HD11  | 1:2:A:ILE:HA    | 1        | 0.2           |
| (3,1539) | 1:2:A:ILE:HD12  | 1:2:A:ILE:HA    | 1        | 0.2           |
| (3,1539) | 1:2:A:ILE:HD13  | 1:2:A:ILE:HA    | 1        | 0.2           |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1  | 22       | 0.2           |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2  | 22       | 0.2           |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1  | 22       | 0.2           |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2  | 22       | 0.2           |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1  | 22       | 0.2           |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2  | 22       | 0.2           |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1  | 29       | 0.2           |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2  | 29       | 0.2           |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1  | 29       | 0.2           |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2  | 29       | 0.2           |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1  | 29       | 0.2           |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2  | 29       | 0.2           |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1  | 31       | 0.2           |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2  | 31       | 0.2           |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1  | 31       | 0.2           |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2  | 31       | 0.2           |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1  | 31       | 0.2           |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2  | 31       | 0.2           |
| (3,1512) | 1:66:A:MET:HE1  | 1:42:A:TRP:HZ3  | 37       | 0.2           |
| (3,1512) | 1:66:A:MET:HE2  | 1:42:A:TRP:HZ3  | 37       | 0.2           |
| (3,1512) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3  | 37       | 0.2           |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA   | 1        | 0.2           |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA   | 1        | 0.2           |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA   | 1        | 0.2           |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA   | 3        | 0.2           |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA   | 3        | 0.2           |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA   | 3        | 0.2           |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA   | 13       | 0.2           |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA   | 13       | 0.2           |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 13       | 0.2           |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 24       | 0.2           |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 24       | 0.2           |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 24       | 0.2           |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 33       | 0.2           |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 33       | 0.2           |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 33       | 0.2           |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 4        | 0.2           |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 4        | 0.2           |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 4        | 0.2           |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 7        | 0.2           |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 7        | 0.2           |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 7        | 0.2           |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 10       | 0.2           |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 10       | 0.2           |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 10       | 0.2           |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 18       | 0.2           |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 18       | 0.2           |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 18       | 0.2           |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 24       | 0.2           |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 24       | 0.2           |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 24       | 0.2           |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 33       | 0.2           |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 33       | 0.2           |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 33       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 1        | 0.2           |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 1        | 0.2           |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 1        | 0.2           |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 3        | 0.2           |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 3        | 0.2           |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 3        | 0.2           |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 6        | 0.2           |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 6        | 0.2           |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 6        | 0.2           |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 10       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 10       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 10       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 12       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 12       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 12       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 13       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 13       | 0.2           |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 13       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 16       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 16       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 16       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 23       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 23       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 23       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 25       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 25       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 25       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 30       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 30       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 30       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 32       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 32       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 32       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 33       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 33       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 33       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 39       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 39       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 39       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 40       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 40       | 0.2           |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 40       | 0.2           |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 1        | 0.2           |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 1        | 0.2           |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 1        | 0.2           |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 12       | 0.2           |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 12       | 0.2           |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 12       | 0.2           |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 19       | 0.2           |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 19       | 0.2           |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 19       | 0.2           |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 21       | 0.2           |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 21       | 0.2           |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 21       | 0.2           |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 25       | 0.2           |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 25       | 0.2           |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 25       | 0.2           |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 26       | 0.2           |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 26       | 0.2           |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H  | 26       | 0.2           |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H  | 30       | 0.2           |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H  | 30       | 0.2           |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H  | 30       | 0.2           |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H  | 36       | 0.2           |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H  | 36       | 0.2           |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H  | 36       | 0.2           |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H  | 38       | 0.2           |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H  | 38       | 0.2           |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H  | 38       | 0.2           |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H  | 6        | 0.2           |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H  | 6        | 0.2           |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H  | 6        | 0.2           |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H  | 22       | 0.2           |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H  | 22       | 0.2           |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H  | 22       | 0.2           |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H  | 23       | 0.2           |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H  | 23       | 0.2           |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H  | 23       | 0.2           |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H  | 37       | 0.2           |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H  | 37       | 0.2           |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H  | 37       | 0.2           |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H  | 1        | 0.2           |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H  | 1        | 0.2           |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H  | 1        | 0.2           |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H  | 3        | 0.2           |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H  | 3        | 0.2           |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H  | 3        | 0.2           |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H  | 6        | 0.2           |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H  | 6        | 0.2           |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H  | 6        | 0.2           |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H  | 12       | 0.2           |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H  | 12       | 0.2           |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H  | 12       | 0.2           |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H  | 19       | 0.2           |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H  | 19       | 0.2           |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H  | 19       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA | 5        | 0.2           |
| (3,1400) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA | 5        | 0.2           |
| (3,1400) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA | 5        | 0.2           |
| (3,1400) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA | 8        | 0.2           |
| (3,1400) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA | 8        | 0.2           |

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| Key      | Atom-1         | Atom-2        | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (3,1400) | 1:95:A:ALA:HB3 | 1:94:A:THR:HA | 8        | 0.2           |
| (3,1400) | 1:95:A:ALA:HB1 | 1:94:A:THR:HA | 10       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB2 | 1:94:A:THR:HA | 10       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB3 | 1:94:A:THR:HA | 10       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB1 | 1:94:A:THR:HA | 13       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB2 | 1:94:A:THR:HA | 13       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB3 | 1:94:A:THR:HA | 13       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB1 | 1:94:A:THR:HA | 14       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB2 | 1:94:A:THR:HA | 14       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB3 | 1:94:A:THR:HA | 14       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB1 | 1:94:A:THR:HA | 18       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB2 | 1:94:A:THR:HA | 18       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB3 | 1:94:A:THR:HA | 18       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB1 | 1:94:A:THR:HA | 23       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB2 | 1:94:A:THR:HA | 23       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB3 | 1:94:A:THR:HA | 23       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB1 | 1:94:A:THR:HA | 25       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB2 | 1:94:A:THR:HA | 25       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB3 | 1:94:A:THR:HA | 25       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB1 | 1:94:A:THR:HA | 26       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB2 | 1:94:A:THR:HA | 26       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB3 | 1:94:A:THR:HA | 26       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB1 | 1:94:A:THR:HA | 27       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB2 | 1:94:A:THR:HA | 27       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB3 | 1:94:A:THR:HA | 27       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB1 | 1:94:A:THR:HA | 30       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB2 | 1:94:A:THR:HA | 30       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB3 | 1:94:A:THR:HA | 30       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB1 | 1:94:A:THR:HA | 31       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB2 | 1:94:A:THR:HA | 31       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB3 | 1:94:A:THR:HA | 31       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB1 | 1:94:A:THR:HA | 32       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB2 | 1:94:A:THR:HA | 32       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB3 | 1:94:A:THR:HA | 32       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB1 | 1:94:A:THR:HA | 33       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB2 | 1:94:A:THR:HA | 33       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB3 | 1:94:A:THR:HA | 33       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB1 | 1:94:A:THR:HA | 34       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB2 | 1:94:A:THR:HA | 34       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB3 | 1:94:A:THR:HA | 34       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB1 | 1:94:A:THR:HA | 35       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB2 | 1:94:A:THR:HA | 35       | 0.2           |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1400) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 35       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 36       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 36       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 36       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 37       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 37       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 37       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 39       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 39       | 0.2           |
| (3,1400) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 39       | 0.2           |
| (3,1391) | 1:91:A:ALA:HB1  | 1:12:A:PHE:HZ  | 6        | 0.2           |
| (3,1391) | 1:91:A:ALA:HB2  | 1:12:A:PHE:HZ  | 6        | 0.2           |
| (3,1391) | 1:91:A:ALA:HB3  | 1:12:A:PHE:HZ  | 6        | 0.2           |
| (3,1391) | 1:91:A:ALA:HB1  | 1:12:A:PHE:HZ  | 7        | 0.2           |
| (3,1391) | 1:91:A:ALA:HB2  | 1:12:A:PHE:HZ  | 7        | 0.2           |
| (3,1391) | 1:91:A:ALA:HB3  | 1:12:A:PHE:HZ  | 7        | 0.2           |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3 | 14       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 12       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 12       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 12       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 13       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 13       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 13       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 21       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 21       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 21       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 24       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 24       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 24       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 27       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 27       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 27       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 29       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 29       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 29       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 30       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 30       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 30       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 32       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 32       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 32       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 38       | 0.2           |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 38       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 38       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 39       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 39       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 39       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 40       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 40       | 0.2           |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 40       | 0.2           |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 1        | 0.2           |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 1        | 0.2           |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 1        | 0.2           |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 5        | 0.2           |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 5        | 0.2           |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 5        | 0.2           |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 6        | 0.2           |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 6        | 0.2           |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 6        | 0.2           |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 21       | 0.2           |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 21       | 0.2           |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 21       | 0.2           |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 24       | 0.2           |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 24       | 0.2           |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 24       | 0.2           |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 34       | 0.2           |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 34       | 0.2           |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 34       | 0.2           |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 39       | 0.2           |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 39       | 0.2           |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 39       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA  | 1        | 0.2           |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA  | 1        | 0.2           |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA  | 1        | 0.2           |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA  | 2        | 0.2           |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA  | 2        | 0.2           |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA  | 2        | 0.2           |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA  | 4        | 0.2           |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA  | 4        | 0.2           |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA  | 4        | 0.2           |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA  | 5        | 0.2           |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA  | 5        | 0.2           |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA  | 5        | 0.2           |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA  | 8        | 0.2           |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA | 8        | 0.2           |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA | 8        | 0.2           |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA | 9        | 0.2           |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA | 9        | 0.2           |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA | 9        | 0.2           |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA | 12       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA | 12       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA | 12       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA | 13       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA | 13       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA | 13       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA | 15       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA | 15       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA | 15       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA | 17       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA | 17       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA | 17       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA | 18       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA | 18       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA | 18       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA | 21       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA | 21       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA | 21       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA | 22       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA | 22       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA | 22       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA | 23       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA | 23       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA | 23       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA | 24       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA | 24       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA | 24       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA | 25       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA | 25       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA | 25       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA | 28       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA | 28       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA | 28       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA | 29       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA | 29       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA | 29       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA | 30       | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 30       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 30       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 31       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 31       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 31       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 32       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 32       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 32       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 33       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 33       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 33       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 34       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 34       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 34       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 35       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 35       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 35       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 36       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 36       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 36       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 37       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 37       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 37       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 38       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 38       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 38       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 39       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 39       | 0.2           |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 39       | 0.2           |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 36       | 0.2           |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 36       | 0.2           |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 36       | 0.2           |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 36       | 0.2           |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 36       | 0.2           |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 36       | 0.2           |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 3        | 0.2           |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 3        | 0.2           |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 3        | 0.2           |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 12       | 0.2           |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 12       | 0.2           |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 12       | 0.2           |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 25       | 0.2           |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 25       | 0.2           |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 25       | 0.2           |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 32       | 0.2           |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 32       | 0.2           |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 32       | 0.2           |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 33       | 0.2           |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 33       | 0.2           |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 33       | 0.2           |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 34       | 0.2           |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 34       | 0.2           |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 34       | 0.2           |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 35       | 0.2           |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 35       | 0.2           |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 35       | 0.2           |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 38       | 0.2           |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 38       | 0.2           |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 38       | 0.2           |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 3        | 0.2           |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 3        | 0.2           |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 3        | 0.2           |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 12       | 0.2           |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 12       | 0.2           |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 12       | 0.2           |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 25       | 0.2           |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 25       | 0.2           |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 25       | 0.2           |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 32       | 0.2           |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 32       | 0.2           |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 32       | 0.2           |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 33       | 0.2           |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 33       | 0.2           |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 33       | 0.2           |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 34       | 0.2           |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 34       | 0.2           |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 34       | 0.2           |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 35       | 0.2           |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 35       | 0.2           |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 35       | 0.2           |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 38       | 0.2           |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 38       | 0.2           |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 38       | 0.2           |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3 | 19       | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 19       | 0.2           |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 19       | 0.2           |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 26       | 0.2           |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 26       | 0.2           |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 26       | 0.2           |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 40       | 0.2           |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 40       | 0.2           |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 40       | 0.2           |
| (3,1230) | 1:101:A:LEU:H   | 1:22:A:SER:HA   | 34       | 0.2           |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 4        | 0.2           |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 11       | 0.2           |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 22       | 0.2           |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 29       | 0.2           |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 8        | 0.2           |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 8        | 0.2           |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 8        | 0.2           |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 7        | 0.2           |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 26       | 0.2           |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 29       | 0.2           |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 31       | 0.2           |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 32       | 0.2           |
| (3,1173) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 8        | 0.2           |
| (3,1173) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 19       | 0.2           |
| (3,1173) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 20       | 0.2           |
| (3,1173) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 25       | 0.2           |
| (3,1173) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 26       | 0.2           |
| (3,1173) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 28       | 0.2           |
| (3,1173) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 30       | 0.2           |
| (3,1173) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 39       | 0.2           |
| (3,1167) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 5        | 0.2           |
| (3,1167) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 14       | 0.2           |
| (3,1167) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 15       | 0.2           |
| (3,1167) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 22       | 0.2           |
| (3,1167) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 23       | 0.2           |
| (3,1167) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 24       | 0.2           |
| (3,1167) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 25       | 0.2           |
| (3,1167) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 31       | 0.2           |
| (3,1167) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 35       | 0.2           |
| (3,1167) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 40       | 0.2           |
| (3,1166) | 1:97:A:LEU:H    | 1:29:A:PHE:HE1  | 3        | 0.2           |
| (3,1166) | 1:97:A:LEU:H    | 1:29:A:PHE:HE2  | 3        | 0.2           |
| (3,1166) | 1:97:A:LEU:H    | 1:29:A:PHE:HE1  | 10       | 0.2           |

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| Key      | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|----------|---------------|----------------|----------|---------------|
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2 | 10       | 0.2           |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1 | 13       | 0.2           |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2 | 13       | 0.2           |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1 | 15       | 0.2           |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2 | 15       | 0.2           |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1 | 21       | 0.2           |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2 | 21       | 0.2           |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1 | 38       | 0.2           |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2 | 38       | 0.2           |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 1        | 0.2           |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 8        | 0.2           |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 9        | 0.2           |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 31       | 0.2           |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 32       | 0.2           |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 34       | 0.2           |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 35       | 0.2           |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 38       | 0.2           |
| (3,970)  | 1:21:A:VAL:H  | 1:20:A:VAL:HB  | 10       | 0.2           |
| (3,970)  | 1:21:A:VAL:H  | 1:20:A:VAL:HB  | 20       | 0.2           |
| (3,968)  | 1:21:A:VAL:H  | 1:99:A:GLY:HA3 | 5        | 0.2           |
| (3,942)  | 1:34:A:SER:H  | 1:12:A:PHE:HA  | 35       | 0.2           |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB  | 6        | 0.2           |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB  | 17       | 0.2           |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB  | 18       | 0.2           |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB  | 35       | 0.2           |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB  | 38       | 0.2           |
| (3,919)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB3 | 8        | 0.2           |
| (3,919)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB3 | 11       | 0.2           |
| (3,919)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB3 | 13       | 0.2           |
| (3,889)  | 1:80:A:SER:H  | 1:43:A:TYR:HB3 | 21       | 0.2           |
| (3,889)  | 1:80:A:SER:H  | 1:43:A:TYR:HB3 | 36       | 0.2           |
| (3,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3  | 22       | 0.2           |
| (3,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3  | 25       | 0.2           |
| (3,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3  | 29       | 0.2           |
| (3,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3  | 36       | 0.2           |
| (3,870)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD2  | 1        | 0.2           |
| (3,870)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD2  | 2        | 0.2           |
| (3,870)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD2  | 13       | 0.2           |
| (3,870)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD2  | 19       | 0.2           |
| (3,849)  | 1:83:A:ALA:H  | 1:91:A:ALA:HB1 | 10       | 0.2           |
| (3,849)  | 1:83:A:ALA:H  | 1:91:A:ALA:HB2 | 10       | 0.2           |
| (3,849)  | 1:83:A:ALA:H  | 1:91:A:ALA:HB3 | 10       | 0.2           |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 20       | 0.2           |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 20       | 0.2           |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 20       | 0.2           |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 2        | 0.2           |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 2        | 0.2           |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 2        | 0.2           |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 7        | 0.2           |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 7        | 0.2           |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 7        | 0.2           |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 8        | 0.2           |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 8        | 0.2           |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 8        | 0.2           |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 15       | 0.2           |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 15       | 0.2           |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 15       | 0.2           |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 21       | 0.2           |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 21       | 0.2           |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 21       | 0.2           |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 25       | 0.2           |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 25       | 0.2           |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 25       | 0.2           |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 30       | 0.2           |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 30       | 0.2           |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 30       | 0.2           |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 40       | 0.2           |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 40       | 0.2           |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 40       | 0.2           |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 9        | 0.2           |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 21       | 0.2           |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 22       | 0.2           |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 34       | 0.2           |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 35       | 0.2           |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 36       | 0.2           |
| (3,786) | 1:6:A:THR:H  | 1:6:A:THR:HG21  | 36       | 0.2           |
| (3,786) | 1:6:A:THR:H  | 1:6:A:THR:HG22  | 36       | 0.2           |
| (3,786) | 1:6:A:THR:H  | 1:6:A:THR:HG23  | 36       | 0.2           |
| (3,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2  | 8        | 0.2           |
| (3,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2  | 9        | 0.2           |
| (3,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2  | 22       | 0.2           |
| (3,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 1        | 0.2           |
| (3,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 5        | 0.2           |
| (3,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 6        | 0.2           |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (3,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 7        | 0.2           |
| (3,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 9        | 0.2           |
| (3,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 11       | 0.2           |
| (3,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 17       | 0.2           |
| (3,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 18       | 0.2           |
| (3,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 21       | 0.2           |
| (3,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 22       | 0.2           |
| (3,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 25       | 0.2           |
| (3,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 27       | 0.2           |
| (3,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 28       | 0.2           |
| (3,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 31       | 0.2           |
| (3,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 32       | 0.2           |
| (3,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 33       | 0.2           |
| (3,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 34       | 0.2           |
| (3,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 35       | 0.2           |
| (3,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 37       | 0.2           |
| (3,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 2        | 0.2           |
| (3,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 11       | 0.2           |
| (3,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 16       | 0.2           |
| (3,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 22       | 0.2           |
| (3,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 30       | 0.2           |
| (3,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 33       | 0.2           |
| (3,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 37       | 0.2           |
| (3,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3  | 5        | 0.2           |
| (3,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3  | 16       | 0.2           |
| (3,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3  | 38       | 0.2           |
| (3,669) | 1:72:A:THR:H  | 1:72:A:THR:HG21 | 17       | 0.2           |
| (3,669) | 1:72:A:THR:H  | 1:72:A:THR:HG22 | 17       | 0.2           |
| (3,669) | 1:72:A:THR:H  | 1:72:A:THR:HG23 | 17       | 0.2           |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 14       | 0.2           |
| (3,590) | 1:3:A:ASP:H   | 1:2:A:ILE:HA    | 30       | 0.2           |
| (3,589) | 1:93:A:SER:H  | 1:92:A:ARG:HG2  | 4        | 0.2           |
| (3,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 3        | 0.2           |
| (3,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2  | 3        | 0.2           |
| (3,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 26       | 0.2           |
| (3,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2  | 26       | 0.2           |
| (3,556) | 1:47:A:THR:H  | 1:48:A:GLU:H    | 1        | 0.2           |
| (3,556) | 1:47:A:THR:H  | 1:48:A:GLU:H    | 7        | 0.2           |
| (3,556) | 1:47:A:THR:H  | 1:48:A:GLU:H    | 12       | 0.2           |
| (3,556) | 1:47:A:THR:H  | 1:48:A:GLU:H    | 13       | 0.2           |
| (3,556) | 1:47:A:THR:H  | 1:48:A:GLU:H    | 15       | 0.2           |
| (3,556) | 1:47:A:THR:H  | 1:48:A:GLU:H    | 17       | 0.2           |

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| Key     | Atom-1       | Atom-2         | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (3,556) | 1:47:A:THR:H | 1:48:A:GLU:H   | 24       | 0.2           |
| (3,556) | 1:47:A:THR:H | 1:48:A:GLU:H   | 27       | 0.2           |
| (3,556) | 1:47:A:THR:H | 1:48:A:GLU:H   | 32       | 0.2           |
| (3,556) | 1:47:A:THR:H | 1:48:A:GLU:H   | 33       | 0.2           |
| (3,556) | 1:47:A:THR:H | 1:48:A:GLU:H   | 35       | 0.2           |
| (3,556) | 1:47:A:THR:H | 1:48:A:GLU:H   | 36       | 0.2           |
| (3,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2 | 1        | 0.2           |
| (3,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2 | 20       | 0.2           |
| (3,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2 | 24       | 0.2           |
| (3,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2 | 33       | 0.2           |
| (3,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2 | 38       | 0.2           |
| (3,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA  | 1        | 0.2           |
| (3,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA  | 8        | 0.2           |
| (3,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA  | 13       | 0.2           |
| (3,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA  | 24       | 0.2           |
| (3,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA  | 38       | 0.2           |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 13       | 0.2           |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2 | 14       | 0.2           |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2 | 28       | 0.2           |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2 | 36       | 0.2           |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H  | 19       | 0.2           |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H  | 20       | 0.2           |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H  | 39       | 0.2           |
| (3,513) | 1:67:A:THR:H | 1:66:A:MET:HG3 | 16       | 0.2           |
| (3,513) | 1:67:A:THR:H | 1:66:A:MET:HG3 | 29       | 0.2           |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2 | 17       | 0.2           |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2 | 38       | 0.2           |
| (3,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2 | 9        | 0.2           |
| (3,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2 | 35       | 0.2           |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA  | 11       | 0.2           |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA  | 14       | 0.2           |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA  | 18       | 0.2           |
| (3,366) | 1:18:A:ASN:H | 1:18:A:ASN:HB3 | 4        | 0.2           |
| (3,366) | 1:18:A:ASN:H | 1:18:A:ASN:HB3 | 11       | 0.2           |
| (3,366) | 1:18:A:ASN:H | 1:18:A:ASN:HB3 | 13       | 0.2           |
| (3,366) | 1:18:A:ASN:H | 1:18:A:ASN:HB3 | 24       | 0.2           |
| (3,366) | 1:18:A:ASN:H | 1:18:A:ASN:HB3 | 25       | 0.2           |
| (3,366) | 1:18:A:ASN:H | 1:18:A:ASN:HB3 | 32       | 0.2           |
| (3,366) | 1:18:A:ASN:H | 1:18:A:ASN:HB3 | 35       | 0.2           |
| (3,366) | 1:18:A:ASN:H | 1:18:A:ASN:HB3 | 36       | 0.2           |
| (3,366) | 1:18:A:ASN:H | 1:18:A:ASN:HB3 | 38       | 0.2           |
| (3,366) | 1:18:A:ASN:H | 1:18:A:ASN:HB3 | 39       | 0.2           |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (3,366) | 1:18:A:ASN:H  | 1:18:A:ASN:HB3  | 40       | 0.2           |
| (3,343) | 1:14:A:LYS:H  | 1:33:A:VAL:HA   | 1        | 0.2           |
| (3,343) | 1:14:A:LYS:H  | 1:33:A:VAL:HA   | 7        | 0.2           |
| (3,343) | 1:14:A:LYS:H  | 1:33:A:VAL:HA   | 8        | 0.2           |
| (3,343) | 1:14:A:LYS:H  | 1:33:A:VAL:HA   | 10       | 0.2           |
| (3,343) | 1:14:A:LYS:H  | 1:33:A:VAL:HA   | 12       | 0.2           |
| (3,343) | 1:14:A:LYS:H  | 1:33:A:VAL:HA   | 31       | 0.2           |
| (3,343) | 1:14:A:LYS:H  | 1:33:A:VAL:HA   | 33       | 0.2           |
| (3,274) | 1:66:A:MET:H  | 1:66:A:MET:HG3  | 28       | 0.2           |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 3        | 0.2           |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 3        | 0.2           |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 3        | 0.2           |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 12       | 0.2           |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 12       | 0.2           |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 12       | 0.2           |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 25       | 0.2           |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 25       | 0.2           |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 25       | 0.2           |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 32       | 0.2           |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 32       | 0.2           |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 32       | 0.2           |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 33       | 0.2           |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 33       | 0.2           |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 33       | 0.2           |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 34       | 0.2           |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 34       | 0.2           |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 34       | 0.2           |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 35       | 0.2           |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 35       | 0.2           |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 35       | 0.2           |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 38       | 0.2           |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 38       | 0.2           |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 38       | 0.2           |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 11       | 0.2           |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 1        | 0.2           |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 8        | 0.2           |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 9        | 0.2           |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 31       | 0.2           |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 32       | 0.2           |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 34       | 0.2           |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 35       | 0.2           |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 38       | 0.2           |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,135)  | 1:39:A:ILE:H   | 1:39:A:ILE:HG13 | 14       | 0.2           |
| (3,135)  | 1:39:A:ILE:H   | 1:39:A:ILE:HG13 | 16       | 0.2           |
| (3,135)  | 1:39:A:ILE:H   | 1:39:A:ILE:HG13 | 22       | 0.2           |
| (3,135)  | 1:39:A:ILE:H   | 1:39:A:ILE:HG13 | 26       | 0.2           |
| (3,135)  | 1:39:A:ILE:H   | 1:39:A:ILE:HG13 | 32       | 0.2           |
| (3,135)  | 1:39:A:ILE:H   | 1:39:A:ILE:HG13 | 34       | 0.2           |
| (3,102)  | 1:22:A:SER:H   | 1:21:A:VAL:HB   | 39       | 0.2           |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 3        | 0.2           |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 3        | 0.2           |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 3        | 0.2           |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 6        | 0.2           |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 6        | 0.2           |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 6        | 0.2           |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 16       | 0.2           |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 16       | 0.2           |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 16       | 0.2           |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 18       | 0.2           |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 18       | 0.2           |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 18       | 0.2           |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 31       | 0.2           |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 31       | 0.2           |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 31       | 0.2           |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 33       | 0.2           |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 33       | 0.2           |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 33       | 0.2           |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 40       | 0.2           |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 40       | 0.2           |
| (3,74)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 40       | 0.2           |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 32       | 0.2           |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 32       | 0.2           |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 35       | 0.2           |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 35       | 0.2           |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 3        | 0.2           |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 3        | 0.2           |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 3        | 0.2           |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 3        | 0.2           |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 3        | 0.2           |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 3        | 0.2           |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 29       | 0.2           |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 29       | 0.2           |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 29       | 0.2           |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 29       | 0.2           |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 29       | 0.2           |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 29       | 0.2           |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 7        | 0.2           |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 7        | 0.2           |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 7        | 0.2           |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 7        | 0.2           |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 4        | 0.2           |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 7        | 0.2           |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 8        | 0.2           |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 26       | 0.2           |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 31       | 0.2           |
| (1,3137) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3  | 34       | 0.2           |
| (1,3137) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 34       | 0.2           |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2  | 35       | 0.2           |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2  | 35       | 0.2           |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 23       | 0.2           |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 23       | 0.2           |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 33       | 0.2           |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 33       | 0.2           |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 34       | 0.2           |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 34       | 0.2           |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 36       | 0.2           |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 36       | 0.2           |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 20       | 0.2           |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 23       | 0.2           |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 25       | 0.2           |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 34       | 0.2           |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 2        | 0.2           |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 2        | 0.2           |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 2        | 0.2           |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 3        | 0.2           |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 3        | 0.2           |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 3        | 0.2           |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 11       | 0.2           |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 11       | 0.2           |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 11       | 0.2           |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 24       | 0.2           |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 24       | 0.2           |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 24       | 0.2           |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 33       | 0.2           |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 33       | 0.2           |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 33       | 0.2           |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 35       | 0.2           |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 35       | 0.2           |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 35       | 0.2           |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 36       | 0.2           |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 36       | 0.2           |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 36       | 0.2           |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 37       | 0.2           |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 37       | 0.2           |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 37       | 0.2           |
| (1,2996) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 17       | 0.2           |
| (1,2996) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 26       | 0.2           |
| (1,2969) | 1:53:A:GLN:HG3 | 1:53:A:GLN:HB2  | 35       | 0.2           |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1  | 34       | 0.2           |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2  | 34       | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 1        | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 2        | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 3        | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 4        | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 5        | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 6        | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 7        | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 8        | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 9        | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 10       | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 11       | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 13       | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 14       | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 15       | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 16       | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 17       | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 18       | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 20       | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 22       | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 23       | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 24       | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 25       | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 26       | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 27       | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 28       | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 29       | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 30       | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 31       | 0.2           |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2867) | 1:92:A:ARG:HD2  | 1:92:A:ARG:HG2 | 33       | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2  | 1:92:A:ARG:HG2 | 34       | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2  | 1:92:A:ARG:HG2 | 35       | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2  | 1:92:A:ARG:HG2 | 36       | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2  | 1:92:A:ARG:HG2 | 37       | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2  | 1:92:A:ARG:HG2 | 38       | 0.2           |
| (1,2867) | 1:92:A:ARG:HD2  | 1:92:A:ARG:HG2 | 40       | 0.2           |
| (1,2802) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HB2 | 14       | 0.2           |
| (1,2802) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HB2 | 15       | 0.2           |
| (1,2802) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HB2 | 23       | 0.2           |
| (1,2802) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HB2 | 29       | 0.2           |
| (1,2802) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HB2 | 32       | 0.2           |
| (1,2802) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HB2 | 36       | 0.2           |
| (1,2802) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HB2 | 40       | 0.2           |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H  | 14       | 0.2           |
| (1,2754) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H   | 7        | 0.2           |
| (1,2754) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H   | 27       | 0.2           |
| (1,2754) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H   | 30       | 0.2           |
| (1,2734) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 2        | 0.2           |
| (1,2734) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 3        | 0.2           |
| (1,2734) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 6        | 0.2           |
| (1,2734) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 7        | 0.2           |
| (1,2734) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 10       | 0.2           |
| (1,2734) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 11       | 0.2           |
| (1,2734) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 13       | 0.2           |
| (1,2734) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 14       | 0.2           |
| (1,2734) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 18       | 0.2           |
| (1,2734) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 20       | 0.2           |
| (1,2734) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 23       | 0.2           |
| (1,2734) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 25       | 0.2           |
| (1,2734) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 26       | 0.2           |
| (1,2734) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 28       | 0.2           |
| (1,2734) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 29       | 0.2           |
| (1,2734) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 30       | 0.2           |
| (1,2734) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 31       | 0.2           |
| (1,2734) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 32       | 0.2           |
| (1,2734) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 33       | 0.2           |
| (1,2734) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 34       | 0.2           |
| (1,2734) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 35       | 0.2           |
| (1,2734) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 36       | 0.2           |
| (1,2734) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 38       | 0.2           |
| (1,2734) | 1:76:A:GLU:HG2  | 1:76:A:GLU:HB2 | 39       | 0.2           |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,2734) | 1:76:A:GLU:HG2 | 1:76:A:GLU:HB2 | 40       | 0.2           |
| (1,2685) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 16       | 0.2           |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 2        | 0.2           |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 3        | 0.2           |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 8        | 0.2           |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 13       | 0.2           |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 18       | 0.2           |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 26       | 0.2           |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 27       | 0.2           |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 28       | 0.2           |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 31       | 0.2           |
| (1,2626) | 1:11:A:GLN:HG2 | 1:11:A:GLN:HB2 | 33       | 0.2           |
| (1,2613) | 1:74:A:ASP:HB2 | 1:74:A:ASP:HA  | 17       | 0.2           |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 8        | 0.2           |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 11       | 0.2           |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 13       | 0.2           |
| (1,2534) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 1        | 0.2           |
| (1,2534) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 19       | 0.2           |
| (1,2534) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 20       | 0.2           |
| (1,2511) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 9        | 0.2           |
| (1,2511) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 12       | 0.2           |
| (1,2511) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 19       | 0.2           |
| (1,2485) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 23       | 0.2           |
| (1,2485) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 29       | 0.2           |
| (1,2485) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 31       | 0.2           |
| (1,2485) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 33       | 0.2           |
| (1,2485) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 34       | 0.2           |
| (1,2485) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 36       | 0.2           |
| (1,2485) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 39       | 0.2           |
| (1,2485) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 40       | 0.2           |
| (1,2431) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 23       | 0.2           |
| (1,2431) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 28       | 0.2           |
| (1,2431) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 29       | 0.2           |
| (1,2402) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 17       | 0.2           |
| (1,2402) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 17       | 0.2           |
| (1,2402) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 17       | 0.2           |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 5        | 0.2           |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 6        | 0.2           |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 7        | 0.2           |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 9        | 0.2           |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 34       | 0.2           |
| (1,2322) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 3        | 0.2           |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,2322) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 7        | 0.2           |
| (1,2322) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 11       | 0.2           |
| (1,2322) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 13       | 0.2           |
| (1,2322) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 26       | 0.2           |
| (1,2286) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 2        | 0.2           |
| (1,2286) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 9        | 0.2           |
| (1,2286) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 10       | 0.2           |
| (1,2286) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 11       | 0.2           |
| (1,2286) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 13       | 0.2           |
| (1,2286) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 17       | 0.2           |
| (1,2286) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 22       | 0.2           |
| (1,2286) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 24       | 0.2           |
| (1,2286) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 25       | 0.2           |
| (1,2286) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 30       | 0.2           |
| (1,2286) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 32       | 0.2           |
| (1,2286) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 34       | 0.2           |
| (1,2286) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 36       | 0.2           |
| (1,2286) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 38       | 0.2           |
| (1,2278) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 12       | 0.2           |
| (1,2250) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1 | 7        | 0.2           |
| (1,2250) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2 | 7        | 0.2           |
| (1,2250) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1 | 12       | 0.2           |
| (1,2250) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2 | 12       | 0.2           |
| (1,2250) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1 | 20       | 0.2           |
| (1,2250) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2 | 20       | 0.2           |
| (1,2250) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1 | 22       | 0.2           |
| (1,2250) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2 | 22       | 0.2           |
| (1,2250) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1 | 24       | 0.2           |
| (1,2250) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2 | 24       | 0.2           |
| (1,2250) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1 | 30       | 0.2           |
| (1,2250) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2 | 30       | 0.2           |
| (1,2236) | 1:18:A:ASN:HB3 | 1:18:A:ASN:H   | 4        | 0.2           |
| (1,2236) | 1:18:A:ASN:HB3 | 1:18:A:ASN:H   | 11       | 0.2           |
| (1,2236) | 1:18:A:ASN:HB3 | 1:18:A:ASN:H   | 13       | 0.2           |
| (1,2236) | 1:18:A:ASN:HB3 | 1:18:A:ASN:H   | 24       | 0.2           |
| (1,2236) | 1:18:A:ASN:HB3 | 1:18:A:ASN:H   | 25       | 0.2           |
| (1,2236) | 1:18:A:ASN:HB3 | 1:18:A:ASN:H   | 32       | 0.2           |
| (1,2236) | 1:18:A:ASN:HB3 | 1:18:A:ASN:H   | 35       | 0.2           |
| (1,2236) | 1:18:A:ASN:HB3 | 1:18:A:ASN:H   | 36       | 0.2           |
| (1,2236) | 1:18:A:ASN:HB3 | 1:18:A:ASN:H   | 38       | 0.2           |
| (1,2236) | 1:18:A:ASN:HB3 | 1:18:A:ASN:H   | 39       | 0.2           |
| (1,2236) | 1:18:A:ASN:HB3 | 1:18:A:ASN:H   | 40       | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 5        | 0.2           |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 7        | 0.2           |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 9        | 0.2           |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 10       | 0.2           |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 25       | 0.2           |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 28       | 0.2           |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 32       | 0.2           |
| (1,2143) | 1:94:A:THR:HB   | 1:78:A:VAL:HG11 | 28       | 0.2           |
| (1,2143) | 1:94:A:THR:HB   | 1:78:A:VAL:HG12 | 28       | 0.2           |
| (1,2143) | 1:94:A:THR:HB   | 1:78:A:VAL:HG13 | 28       | 0.2           |
| (1,2099) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HA   | 36       | 0.2           |
| (1,2099) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HA   | 36       | 0.2           |
| (1,2099) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HA   | 36       | 0.2           |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 31       | 0.2           |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 31       | 0.2           |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 31       | 0.2           |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD11 | 5        | 0.2           |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD12 | 5        | 0.2           |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD13 | 5        | 0.2           |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD11 | 5        | 0.2           |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD12 | 5        | 0.2           |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD13 | 5        | 0.2           |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD11 | 5        | 0.2           |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD12 | 5        | 0.2           |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD13 | 5        | 0.2           |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD11 | 14       | 0.2           |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD12 | 14       | 0.2           |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD13 | 14       | 0.2           |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD11 | 14       | 0.2           |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD12 | 14       | 0.2           |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD13 | 14       | 0.2           |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD11 | 14       | 0.2           |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD12 | 14       | 0.2           |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD13 | 14       | 0.2           |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3  | 1        | 0.2           |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3  | 1        | 0.2           |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3  | 1        | 0.2           |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3  | 5        | 0.2           |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3  | 5        | 0.2           |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3  | 5        | 0.2           |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3  | 6        | 0.2           |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3  | 6        | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3  | 6        | 0.2           |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3  | 11       | 0.2           |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3  | 11       | 0.2           |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3  | 11       | 0.2           |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1  | 35       | 0.2           |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2  | 35       | 0.2           |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1  | 35       | 0.2           |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2  | 35       | 0.2           |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1  | 35       | 0.2           |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2  | 35       | 0.2           |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 8        | 0.2           |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 8        | 0.2           |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 8        | 0.2           |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 12       | 0.2           |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 12       | 0.2           |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 12       | 0.2           |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3  | 2        | 0.2           |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3  | 2        | 0.2           |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3  | 2        | 0.2           |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3  | 3        | 0.2           |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3  | 3        | 0.2           |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3  | 3        | 0.2           |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3  | 4        | 0.2           |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3  | 4        | 0.2           |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3  | 4        | 0.2           |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3  | 8        | 0.2           |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3  | 8        | 0.2           |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3  | 8        | 0.2           |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3  | 14       | 0.2           |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3  | 14       | 0.2           |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3  | 14       | 0.2           |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3  | 28       | 0.2           |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3  | 28       | 0.2           |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3  | 28       | 0.2           |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 17       | 0.2           |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 4        | 0.2           |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 4        | 0.2           |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 4        | 0.2           |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 4        | 0.2           |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 4        | 0.2           |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 4        | 0.2           |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 4        | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 4        | 0.2           |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 4        | 0.2           |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 16       | 0.2           |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 16       | 0.2           |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 16       | 0.2           |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 16       | 0.2           |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 16       | 0.2           |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 16       | 0.2           |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 16       | 0.2           |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 16       | 0.2           |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 16       | 0.2           |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD11 | 18       | 0.2           |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD12 | 18       | 0.2           |
| (1,1910) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD13 | 18       | 0.2           |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD11 | 18       | 0.2           |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD12 | 18       | 0.2           |
| (1,1910) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD13 | 18       | 0.2           |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD11 | 18       | 0.2           |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD12 | 18       | 0.2           |
| (1,1910) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD13 | 18       | 0.2           |
| (1,1904) | 1:66:A:MET:HE1  | 1:43:A:TYR:H    | 10       | 0.2           |
| (1,1904) | 1:66:A:MET:HE2  | 1:43:A:TYR:H    | 10       | 0.2           |
| (1,1904) | 1:66:A:MET:HE3  | 1:43:A:TYR:H    | 10       | 0.2           |
| (1,1853) | 1:27:A:ALA:HB1  | 1:28:A:THR:H    | 8        | 0.2           |
| (1,1853) | 1:27:A:ALA:HB2  | 1:28:A:THR:H    | 8        | 0.2           |
| (1,1853) | 1:27:A:ALA:HB3  | 1:28:A:THR:H    | 8        | 0.2           |
| (1,1853) | 1:27:A:ALA:HB1  | 1:28:A:THR:H    | 33       | 0.2           |
| (1,1853) | 1:27:A:ALA:HB2  | 1:28:A:THR:H    | 33       | 0.2           |
| (1,1853) | 1:27:A:ALA:HB3  | 1:28:A:THR:H    | 33       | 0.2           |
| (1,1825) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 3        | 0.2           |
| (1,1825) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 4        | 0.2           |
| (1,1825) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 8        | 0.2           |
| (1,1825) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 9        | 0.2           |
| (1,1825) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 12       | 0.2           |
| (1,1825) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 14       | 0.2           |
| (1,1825) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 19       | 0.2           |
| (1,1825) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 20       | 0.2           |
| (1,1825) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 28       | 0.2           |
| (1,1812) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 3        | 0.2           |
| (1,1812) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 4        | 0.2           |
| (1,1812) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 8        | 0.2           |
| (1,1812) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 9        | 0.2           |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1812) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 12       | 0.2           |
| (1,1812) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 14       | 0.2           |
| (1,1812) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 19       | 0.2           |
| (1,1812) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 20       | 0.2           |
| (1,1812) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 28       | 0.2           |
| (1,1778) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 39       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 2        | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 3        | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 5        | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 6        | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 7        | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 9        | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 10       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 11       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 12       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 13       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 14       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 15       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 16       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 17       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 18       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 19       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 20       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 21       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 22       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 23       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 24       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 25       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 26       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 27       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 28       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 29       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 30       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 31       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 32       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 33       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 34       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 35       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 36       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 37       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 38       | 0.2           |
| (1,1740) | 1:51:A:GLU:HG2 | 1:51:A:GLU:HB2 | 39       | 0.2           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1740) | 1:51:A:GLU:HG2   | 1:51:A:GLU:HB2  | 40       | 0.2           |
| (1,1728) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H    | 2        | 0.2           |
| (1,1728) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H    | 5        | 0.2           |
| (1,1728) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H    | 9        | 0.2           |
| (1,1728) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H    | 11       | 0.2           |
| (1,1728) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H    | 15       | 0.2           |
| (1,1728) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H    | 16       | 0.2           |
| (1,1728) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H    | 34       | 0.2           |
| (1,1728) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H    | 37       | 0.2           |
| (1,1728) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H    | 39       | 0.2           |
| (1,1717) | 1:38:A:ALA:HB1   | 1:33:A:VAL:HG11 | 11       | 0.2           |
| (1,1717) | 1:38:A:ALA:HB1   | 1:33:A:VAL:HG12 | 11       | 0.2           |
| (1,1717) | 1:38:A:ALA:HB1   | 1:33:A:VAL:HG13 | 11       | 0.2           |
| (1,1717) | 1:38:A:ALA:HB2   | 1:33:A:VAL:HG11 | 11       | 0.2           |
| (1,1717) | 1:38:A:ALA:HB2   | 1:33:A:VAL:HG12 | 11       | 0.2           |
| (1,1717) | 1:38:A:ALA:HB2   | 1:33:A:VAL:HG13 | 11       | 0.2           |
| (1,1717) | 1:38:A:ALA:HB3   | 1:33:A:VAL:HG11 | 11       | 0.2           |
| (1,1717) | 1:38:A:ALA:HB3   | 1:33:A:VAL:HG12 | 11       | 0.2           |
| (1,1717) | 1:38:A:ALA:HB3   | 1:33:A:VAL:HG13 | 11       | 0.2           |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 1        | 0.2           |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 1        | 0.2           |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 1        | 0.2           |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 2        | 0.2           |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 2        | 0.2           |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 2        | 0.2           |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 4        | 0.2           |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 4        | 0.2           |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 4        | 0.2           |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 6        | 0.2           |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 6        | 0.2           |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 6        | 0.2           |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 7        | 0.2           |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 7        | 0.2           |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 7        | 0.2           |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 17       | 0.2           |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 17       | 0.2           |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 17       | 0.2           |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 18       | 0.2           |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 18       | 0.2           |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 18       | 0.2           |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 20       | 0.2           |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 20       | 0.2           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 20       | 0.2           |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 22       | 0.2           |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 22       | 0.2           |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 22       | 0.2           |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 37       | 0.2           |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 37       | 0.2           |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 37       | 0.2           |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 39       | 0.2           |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 39       | 0.2           |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 39       | 0.2           |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 40       | 0.2           |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 40       | 0.2           |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 40       | 0.2           |
| (1,1678) | 1:85:A:LEU:HD11  | 1:85:A:LEU:HA   | 18       | 0.2           |
| (1,1678) | 1:85:A:LEU:HD12  | 1:85:A:LEU:HA   | 18       | 0.2           |
| (1,1678) | 1:85:A:LEU:HD13  | 1:85:A:LEU:HA   | 18       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG21  | 1:16:A:ILE:HG21 | 2        | 0.2           |
| (1,1639) | 1:81:A:VAL:HG21  | 1:16:A:ILE:HG22 | 2        | 0.2           |
| (1,1639) | 1:81:A:VAL:HG21  | 1:16:A:ILE:HG23 | 2        | 0.2           |
| (1,1639) | 1:81:A:VAL:HG22  | 1:16:A:ILE:HG21 | 2        | 0.2           |
| (1,1639) | 1:81:A:VAL:HG22  | 1:16:A:ILE:HG22 | 2        | 0.2           |
| (1,1639) | 1:81:A:VAL:HG22  | 1:16:A:ILE:HG23 | 2        | 0.2           |
| (1,1639) | 1:81:A:VAL:HG23  | 1:16:A:ILE:HG21 | 2        | 0.2           |
| (1,1639) | 1:81:A:VAL:HG23  | 1:16:A:ILE:HG22 | 2        | 0.2           |
| (1,1639) | 1:81:A:VAL:HG23  | 1:16:A:ILE:HG23 | 2        | 0.2           |
| (1,1639) | 1:81:A:VAL:HG21  | 1:16:A:ILE:HG21 | 3        | 0.2           |
| (1,1639) | 1:81:A:VAL:HG21  | 1:16:A:ILE:HG22 | 3        | 0.2           |
| (1,1639) | 1:81:A:VAL:HG21  | 1:16:A:ILE:HG23 | 3        | 0.2           |
| (1,1639) | 1:81:A:VAL:HG22  | 1:16:A:ILE:HG21 | 3        | 0.2           |
| (1,1639) | 1:81:A:VAL:HG22  | 1:16:A:ILE:HG22 | 3        | 0.2           |
| (1,1639) | 1:81:A:VAL:HG22  | 1:16:A:ILE:HG23 | 3        | 0.2           |
| (1,1639) | 1:81:A:VAL:HG23  | 1:16:A:ILE:HG21 | 3        | 0.2           |
| (1,1639) | 1:81:A:VAL:HG23  | 1:16:A:ILE:HG22 | 3        | 0.2           |
| (1,1639) | 1:81:A:VAL:HG23  | 1:16:A:ILE:HG23 | 3        | 0.2           |
| (1,1639) | 1:81:A:VAL:HG21  | 1:16:A:ILE:HG21 | 7        | 0.2           |
| (1,1639) | 1:81:A:VAL:HG21  | 1:16:A:ILE:HG22 | 7        | 0.2           |
| (1,1639) | 1:81:A:VAL:HG21  | 1:16:A:ILE:HG23 | 7        | 0.2           |
| (1,1639) | 1:81:A:VAL:HG22  | 1:16:A:ILE:HG21 | 7        | 0.2           |
| (1,1639) | 1:81:A:VAL:HG22  | 1:16:A:ILE:HG22 | 7        | 0.2           |
| (1,1639) | 1:81:A:VAL:HG22  | 1:16:A:ILE:HG23 | 7        | 0.2           |
| (1,1639) | 1:81:A:VAL:HG23  | 1:16:A:ILE:HG21 | 7        | 0.2           |
| (1,1639) | 1:81:A:VAL:HG23  | 1:16:A:ILE:HG22 | 7        | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 7        | 0.2           |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 24       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 24       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 24       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 24       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 24       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 24       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 24       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 24       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 24       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 26       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 26       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 26       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 26       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 26       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 26       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 26       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 26       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 26       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 27       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 27       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 27       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 27       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 27       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 27       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 27       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 27       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 27       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 37       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 37       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 37       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 37       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 37       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 37       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 37       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 37       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 37       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 38       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 38       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 38       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 38       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 38       | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 38       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 38       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 38       | 0.2           |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 38       | 0.2           |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 9        | 0.2           |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 9        | 0.2           |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 9        | 0.2           |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 17       | 0.2           |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 17       | 0.2           |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 17       | 0.2           |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 20       | 0.2           |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 20       | 0.2           |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 20       | 0.2           |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 21       | 0.2           |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 21       | 0.2           |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 21       | 0.2           |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 30       | 0.2           |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 30       | 0.2           |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 30       | 0.2           |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 32       | 0.2           |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 32       | 0.2           |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 32       | 0.2           |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 32       | 0.2           |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 32       | 0.2           |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 32       | 0.2           |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 1        | 0.2           |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 1        | 0.2           |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 1        | 0.2           |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 12       | 0.2           |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 12       | 0.2           |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 12       | 0.2           |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 14       | 0.2           |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 14       | 0.2           |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 14       | 0.2           |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 15       | 0.2           |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 15       | 0.2           |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 15       | 0.2           |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 19       | 0.2           |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 19       | 0.2           |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 19       | 0.2           |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 27       | 0.2           |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 27       | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 27       | 0.2           |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 28       | 0.2           |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 28       | 0.2           |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 28       | 0.2           |
| (1,1535) | 1:2:A:ILE:HD11  | 1:2:A:ILE:HA    | 1        | 0.2           |
| (1,1535) | 1:2:A:ILE:HD12  | 1:2:A:ILE:HA    | 1        | 0.2           |
| (1,1535) | 1:2:A:ILE:HD13  | 1:2:A:ILE:HA    | 1        | 0.2           |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1  | 22       | 0.2           |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2  | 22       | 0.2           |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1  | 22       | 0.2           |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2  | 22       | 0.2           |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1  | 22       | 0.2           |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2  | 22       | 0.2           |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1  | 29       | 0.2           |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2  | 29       | 0.2           |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1  | 29       | 0.2           |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2  | 29       | 0.2           |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1  | 29       | 0.2           |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2  | 29       | 0.2           |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1  | 31       | 0.2           |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2  | 31       | 0.2           |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1  | 31       | 0.2           |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2  | 31       | 0.2           |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1  | 31       | 0.2           |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2  | 31       | 0.2           |
| (1,1508) | 1:66:A:MET:HE1  | 1:42:A:TRP:HZ3  | 37       | 0.2           |
| (1,1508) | 1:66:A:MET:HE2  | 1:42:A:TRP:HZ3  | 37       | 0.2           |
| (1,1508) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3  | 37       | 0.2           |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA   | 1        | 0.2           |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA   | 1        | 0.2           |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA   | 1        | 0.2           |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA   | 3        | 0.2           |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA   | 3        | 0.2           |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA   | 3        | 0.2           |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA   | 13       | 0.2           |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA   | 13       | 0.2           |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA   | 13       | 0.2           |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA   | 24       | 0.2           |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA   | 24       | 0.2           |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA   | 24       | 0.2           |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA   | 33       | 0.2           |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA   | 33       | 0.2           |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 33       | 0.2           |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 4        | 0.2           |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 4        | 0.2           |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 4        | 0.2           |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 7        | 0.2           |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 7        | 0.2           |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 7        | 0.2           |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 10       | 0.2           |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 10       | 0.2           |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 10       | 0.2           |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 18       | 0.2           |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 18       | 0.2           |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 18       | 0.2           |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 24       | 0.2           |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 24       | 0.2           |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 24       | 0.2           |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 33       | 0.2           |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 33       | 0.2           |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 33       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 1        | 0.2           |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 1        | 0.2           |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 1        | 0.2           |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 3        | 0.2           |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 3        | 0.2           |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 3        | 0.2           |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 6        | 0.2           |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 6        | 0.2           |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 6        | 0.2           |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 10       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 10       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 10       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 12       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 12       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 12       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 13       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 13       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 13       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 16       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 16       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 16       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 23       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 23       | 0.2           |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 23       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 25       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 25       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 25       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 30       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 30       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 30       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 32       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 32       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 32       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 33       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 33       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 33       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 39       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 39       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 39       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 40       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 40       | 0.2           |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 40       | 0.2           |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 1        | 0.2           |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 1        | 0.2           |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 1        | 0.2           |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 12       | 0.2           |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 12       | 0.2           |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 12       | 0.2           |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 19       | 0.2           |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 19       | 0.2           |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 19       | 0.2           |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 21       | 0.2           |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 21       | 0.2           |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 21       | 0.2           |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 25       | 0.2           |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 25       | 0.2           |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 25       | 0.2           |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 26       | 0.2           |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 26       | 0.2           |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 26       | 0.2           |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 30       | 0.2           |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 30       | 0.2           |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 30       | 0.2           |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 36       | 0.2           |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 36       | 0.2           |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H  | 36       | 0.2           |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H  | 38       | 0.2           |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H  | 38       | 0.2           |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H  | 38       | 0.2           |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H  | 6        | 0.2           |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H  | 6        | 0.2           |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H  | 6        | 0.2           |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H  | 22       | 0.2           |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H  | 22       | 0.2           |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H  | 22       | 0.2           |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H  | 23       | 0.2           |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H  | 23       | 0.2           |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H  | 23       | 0.2           |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H  | 37       | 0.2           |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H  | 37       | 0.2           |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H  | 37       | 0.2           |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H  | 1        | 0.2           |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H  | 1        | 0.2           |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H  | 1        | 0.2           |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H  | 3        | 0.2           |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H  | 3        | 0.2           |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H  | 3        | 0.2           |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H  | 6        | 0.2           |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H  | 6        | 0.2           |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H  | 6        | 0.2           |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H  | 12       | 0.2           |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H  | 12       | 0.2           |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H  | 12       | 0.2           |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H  | 19       | 0.2           |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H  | 19       | 0.2           |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H  | 19       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA | 5        | 0.2           |
| (1,1396) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA | 5        | 0.2           |
| (1,1396) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA | 5        | 0.2           |
| (1,1396) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA | 8        | 0.2           |
| (1,1396) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA | 8        | 0.2           |
| (1,1396) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA | 8        | 0.2           |
| (1,1396) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA | 10       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA | 10       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA | 10       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA | 13       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA | 13       | 0.2           |

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| Key      | Atom-1         | Atom-2        | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (1,1396) | 1:95:A:ALA:HB3 | 1:94:A:THR:HA | 13       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB1 | 1:94:A:THR:HA | 14       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB2 | 1:94:A:THR:HA | 14       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB3 | 1:94:A:THR:HA | 14       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB1 | 1:94:A:THR:HA | 18       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB2 | 1:94:A:THR:HA | 18       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB3 | 1:94:A:THR:HA | 18       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB1 | 1:94:A:THR:HA | 23       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB2 | 1:94:A:THR:HA | 23       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB3 | 1:94:A:THR:HA | 23       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB1 | 1:94:A:THR:HA | 25       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB2 | 1:94:A:THR:HA | 25       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB3 | 1:94:A:THR:HA | 25       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB1 | 1:94:A:THR:HA | 26       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB2 | 1:94:A:THR:HA | 26       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB3 | 1:94:A:THR:HA | 26       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB1 | 1:94:A:THR:HA | 27       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB2 | 1:94:A:THR:HA | 27       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB3 | 1:94:A:THR:HA | 27       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB1 | 1:94:A:THR:HA | 30       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB2 | 1:94:A:THR:HA | 30       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB3 | 1:94:A:THR:HA | 30       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB1 | 1:94:A:THR:HA | 31       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB2 | 1:94:A:THR:HA | 31       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB3 | 1:94:A:THR:HA | 31       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB1 | 1:94:A:THR:HA | 32       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB2 | 1:94:A:THR:HA | 32       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB3 | 1:94:A:THR:HA | 32       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB1 | 1:94:A:THR:HA | 33       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB2 | 1:94:A:THR:HA | 33       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB3 | 1:94:A:THR:HA | 33       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB1 | 1:94:A:THR:HA | 34       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB2 | 1:94:A:THR:HA | 34       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB3 | 1:94:A:THR:HA | 34       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB1 | 1:94:A:THR:HA | 35       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB2 | 1:94:A:THR:HA | 35       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB3 | 1:94:A:THR:HA | 35       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB1 | 1:94:A:THR:HA | 36       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB2 | 1:94:A:THR:HA | 36       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB3 | 1:94:A:THR:HA | 36       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB1 | 1:94:A:THR:HA | 37       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB2 | 1:94:A:THR:HA | 37       | 0.2           |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1396) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 37       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 39       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 39       | 0.2           |
| (1,1396) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 39       | 0.2           |
| (1,1387) | 1:91:A:ALA:HB1  | 1:12:A:PHE:HZ  | 6        | 0.2           |
| (1,1387) | 1:91:A:ALA:HB2  | 1:12:A:PHE:HZ  | 6        | 0.2           |
| (1,1387) | 1:91:A:ALA:HB3  | 1:12:A:PHE:HZ  | 6        | 0.2           |
| (1,1387) | 1:91:A:ALA:HB1  | 1:12:A:PHE:HZ  | 7        | 0.2           |
| (1,1387) | 1:91:A:ALA:HB2  | 1:12:A:PHE:HZ  | 7        | 0.2           |
| (1,1387) | 1:91:A:ALA:HB3  | 1:12:A:PHE:HZ  | 7        | 0.2           |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3 | 14       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 12       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 12       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 12       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 13       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 13       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 13       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 21       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 21       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 21       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 24       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 24       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 24       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 27       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 27       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 27       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 29       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 29       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 29       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 30       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 30       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 30       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 32       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 32       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 32       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 38       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 38       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 38       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 39       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 39       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 39       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 40       | 0.2           |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 40       | 0.2           |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 40       | 0.2           |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 1        | 0.2           |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 1        | 0.2           |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 1        | 0.2           |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 5        | 0.2           |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 5        | 0.2           |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 5        | 0.2           |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 6        | 0.2           |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 6        | 0.2           |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 6        | 0.2           |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 21       | 0.2           |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 21       | 0.2           |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 21       | 0.2           |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 24       | 0.2           |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 24       | 0.2           |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 24       | 0.2           |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 34       | 0.2           |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 34       | 0.2           |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 34       | 0.2           |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 39       | 0.2           |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 39       | 0.2           |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 39       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA  | 1        | 0.2           |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA  | 1        | 0.2           |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA  | 1        | 0.2           |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA  | 2        | 0.2           |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA  | 2        | 0.2           |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA  | 2        | 0.2           |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA  | 4        | 0.2           |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA  | 4        | 0.2           |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA  | 4        | 0.2           |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA  | 5        | 0.2           |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA  | 5        | 0.2           |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA  | 5        | 0.2           |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA  | 8        | 0.2           |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA  | 8        | 0.2           |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA  | 8        | 0.2           |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA  | 9        | 0.2           |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA  | 9        | 0.2           |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA  | 9        | 0.2           |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA  | 12       | 0.2           |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA | 12       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA | 12       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA | 13       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA | 13       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA | 13       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA | 15       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA | 15       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA | 15       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA | 17       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA | 17       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA | 17       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA | 18       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA | 18       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA | 18       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA | 21       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA | 21       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA | 21       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA | 22       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA | 22       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA | 22       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA | 23       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA | 23       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA | 23       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA | 24       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA | 24       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA | 24       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA | 25       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA | 25       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA | 25       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA | 28       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA | 28       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA | 28       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA | 29       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA | 29       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA | 29       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA | 30       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA | 30       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA | 30       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA | 31       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA | 31       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA | 31       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA | 32       | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 32       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 32       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 33       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 33       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 33       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 34       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 34       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 34       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 35       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 35       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 35       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 36       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 36       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 36       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 37       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 37       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 37       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 38       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 38       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 38       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 39       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 39       | 0.2           |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 39       | 0.2           |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 36       | 0.2           |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 36       | 0.2           |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 36       | 0.2           |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 36       | 0.2           |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 36       | 0.2           |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 36       | 0.2           |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 3        | 0.2           |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 3        | 0.2           |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 3        | 0.2           |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 12       | 0.2           |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 12       | 0.2           |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 12       | 0.2           |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 25       | 0.2           |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 25       | 0.2           |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 25       | 0.2           |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 32       | 0.2           |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 32       | 0.2           |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 32       | 0.2           |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 33       | 0.2           |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 33       | 0.2           |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 33       | 0.2           |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 34       | 0.2           |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 34       | 0.2           |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 34       | 0.2           |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 35       | 0.2           |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 35       | 0.2           |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 35       | 0.2           |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 38       | 0.2           |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 38       | 0.2           |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 38       | 0.2           |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 3        | 0.2           |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 3        | 0.2           |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 3        | 0.2           |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 12       | 0.2           |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 12       | 0.2           |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 12       | 0.2           |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 25       | 0.2           |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 25       | 0.2           |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 25       | 0.2           |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 32       | 0.2           |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 32       | 0.2           |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 32       | 0.2           |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 33       | 0.2           |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 33       | 0.2           |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 33       | 0.2           |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 34       | 0.2           |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 34       | 0.2           |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 34       | 0.2           |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 35       | 0.2           |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 35       | 0.2           |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 35       | 0.2           |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 38       | 0.2           |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 38       | 0.2           |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 38       | 0.2           |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3 | 19       | 0.2           |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3 | 19       | 0.2           |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3 | 19       | 0.2           |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3 | 26       | 0.2           |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3 | 26       | 0.2           |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3 | 26       | 0.2           |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3 | 40       | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 40       | 0.2           |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 40       | 0.2           |
| (1,1226) | 1:101:A:LEU:H   | 1:22:A:SER:HA   | 34       | 0.2           |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 4        | 0.2           |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 11       | 0.2           |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 22       | 0.2           |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 29       | 0.2           |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 8        | 0.2           |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 8        | 0.2           |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 8        | 0.2           |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 7        | 0.2           |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 26       | 0.2           |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 29       | 0.2           |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 31       | 0.2           |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 32       | 0.2           |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 8        | 0.2           |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 19       | 0.2           |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 20       | 0.2           |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 25       | 0.2           |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 26       | 0.2           |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 28       | 0.2           |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 30       | 0.2           |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 39       | 0.2           |
| (1,1163) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 5        | 0.2           |
| (1,1163) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 14       | 0.2           |
| (1,1163) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 15       | 0.2           |
| (1,1163) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 22       | 0.2           |
| (1,1163) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 23       | 0.2           |
| (1,1163) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 24       | 0.2           |
| (1,1163) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 25       | 0.2           |
| (1,1163) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 31       | 0.2           |
| (1,1163) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 35       | 0.2           |
| (1,1163) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 40       | 0.2           |
| (1,1162) | 1:97:A:LEU:H    | 1:29:A:PHE:HE1  | 3        | 0.2           |
| (1,1162) | 1:97:A:LEU:H    | 1:29:A:PHE:HE2  | 3        | 0.2           |
| (1,1162) | 1:97:A:LEU:H    | 1:29:A:PHE:HE1  | 10       | 0.2           |
| (1,1162) | 1:97:A:LEU:H    | 1:29:A:PHE:HE2  | 10       | 0.2           |
| (1,1162) | 1:97:A:LEU:H    | 1:29:A:PHE:HE1  | 13       | 0.2           |
| (1,1162) | 1:97:A:LEU:H    | 1:29:A:PHE:HE2  | 13       | 0.2           |
| (1,1162) | 1:97:A:LEU:H    | 1:29:A:PHE:HE1  | 15       | 0.2           |
| (1,1162) | 1:97:A:LEU:H    | 1:29:A:PHE:HE2  | 15       | 0.2           |
| (1,1162) | 1:97:A:LEU:H    | 1:29:A:PHE:HE1  | 21       | 0.2           |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 21       | 0.2           |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 38       | 0.2           |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 38       | 0.2           |
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 1        | 0.2           |
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 8        | 0.2           |
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 9        | 0.2           |
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 31       | 0.2           |
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 32       | 0.2           |
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 34       | 0.2           |
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 35       | 0.2           |
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 38       | 0.2           |
| (1,969)  | 1:21:A:VAL:H  | 1:20:A:VAL:HB   | 10       | 0.2           |
| (1,969)  | 1:21:A:VAL:H  | 1:20:A:VAL:HB   | 20       | 0.2           |
| (1,967)  | 1:21:A:VAL:H  | 1:99:A:GLY:HA3  | 5        | 0.2           |
| (1,941)  | 1:34:A:SER:H  | 1:12:A:PHE:HA   | 35       | 0.2           |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 6        | 0.2           |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 17       | 0.2           |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 18       | 0.2           |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 35       | 0.2           |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 38       | 0.2           |
| (1,918)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB3  | 8        | 0.2           |
| (1,918)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB3  | 11       | 0.2           |
| (1,918)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB3  | 13       | 0.2           |
| (1,888)  | 1:80:A:SER:H  | 1:43:A:TYR:HB3  | 21       | 0.2           |
| (1,888)  | 1:80:A:SER:H  | 1:43:A:TYR:HB3  | 36       | 0.2           |
| (1,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3   | 22       | 0.2           |
| (1,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3   | 25       | 0.2           |
| (1,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3   | 29       | 0.2           |
| (1,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3   | 36       | 0.2           |
| (1,870)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD2   | 1        | 0.2           |
| (1,870)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD2   | 2        | 0.2           |
| (1,870)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD2   | 13       | 0.2           |
| (1,870)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD2   | 19       | 0.2           |
| (1,849)  | 1:83:A:ALA:H  | 1:91:A:ALA:HB1  | 10       | 0.2           |
| (1,849)  | 1:83:A:ALA:H  | 1:91:A:ALA:HB2  | 10       | 0.2           |
| (1,849)  | 1:83:A:ALA:H  | 1:91:A:ALA:HB3  | 10       | 0.2           |
| (1,849)  | 1:83:A:ALA:H  | 1:91:A:ALA:HB1  | 20       | 0.2           |
| (1,849)  | 1:83:A:ALA:H  | 1:91:A:ALA:HB2  | 20       | 0.2           |
| (1,849)  | 1:83:A:ALA:H  | 1:91:A:ALA:HB3  | 20       | 0.2           |
| (1,814)  | 1:25:A:GLN:H  | 1:71:A:VAL:HG21 | 2        | 0.2           |
| (1,814)  | 1:25:A:GLN:H  | 1:71:A:VAL:HG22 | 2        | 0.2           |
| (1,814)  | 1:25:A:GLN:H  | 1:71:A:VAL:HG23 | 2        | 0.2           |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 7        | 0.2           |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 7        | 0.2           |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 7        | 0.2           |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 8        | 0.2           |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 8        | 0.2           |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 8        | 0.2           |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 15       | 0.2           |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 15       | 0.2           |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 15       | 0.2           |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 21       | 0.2           |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 21       | 0.2           |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 21       | 0.2           |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 25       | 0.2           |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 25       | 0.2           |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 25       | 0.2           |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 30       | 0.2           |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 30       | 0.2           |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 30       | 0.2           |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 40       | 0.2           |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 40       | 0.2           |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 40       | 0.2           |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 9        | 0.2           |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 21       | 0.2           |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 22       | 0.2           |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 34       | 0.2           |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 35       | 0.2           |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 36       | 0.2           |
| (1,786) | 1:6:A:THR:H  | 1:6:A:THR:HG21  | 36       | 0.2           |
| (1,786) | 1:6:A:THR:H  | 1:6:A:THR:HG22  | 36       | 0.2           |
| (1,786) | 1:6:A:THR:H  | 1:6:A:THR:HG23  | 36       | 0.2           |
| (1,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2  | 8        | 0.2           |
| (1,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2  | 9        | 0.2           |
| (1,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2  | 22       | 0.2           |
| (1,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 1        | 0.2           |
| (1,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 5        | 0.2           |
| (1,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 6        | 0.2           |
| (1,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 7        | 0.2           |
| (1,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 9        | 0.2           |
| (1,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 11       | 0.2           |
| (1,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 17       | 0.2           |
| (1,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 18       | 0.2           |
| (1,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 21       | 0.2           |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 22       | 0.2           |
| (1,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 25       | 0.2           |
| (1,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 27       | 0.2           |
| (1,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 28       | 0.2           |
| (1,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 31       | 0.2           |
| (1,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 32       | 0.2           |
| (1,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 33       | 0.2           |
| (1,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 34       | 0.2           |
| (1,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 35       | 0.2           |
| (1,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 37       | 0.2           |
| (1,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 2        | 0.2           |
| (1,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 11       | 0.2           |
| (1,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 16       | 0.2           |
| (1,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 22       | 0.2           |
| (1,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 30       | 0.2           |
| (1,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 33       | 0.2           |
| (1,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 37       | 0.2           |
| (1,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3  | 5        | 0.2           |
| (1,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3  | 16       | 0.2           |
| (1,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3  | 38       | 0.2           |
| (1,669) | 1:72:A:THR:H  | 1:72:A:THR:HG21 | 17       | 0.2           |
| (1,669) | 1:72:A:THR:H  | 1:72:A:THR:HG22 | 17       | 0.2           |
| (1,669) | 1:72:A:THR:H  | 1:72:A:THR:HG23 | 17       | 0.2           |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 14       | 0.2           |
| (1,590) | 1:3:A:ASP:H   | 1:2:A:ILE:HA    | 30       | 0.2           |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 3        | 0.2           |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2  | 3        | 0.2           |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 26       | 0.2           |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2  | 26       | 0.2           |
| (1,556) | 1:47:A:THR:H  | 1:48:A:GLU:H    | 1        | 0.2           |
| (1,556) | 1:47:A:THR:H  | 1:48:A:GLU:H    | 7        | 0.2           |
| (1,556) | 1:47:A:THR:H  | 1:48:A:GLU:H    | 12       | 0.2           |
| (1,556) | 1:47:A:THR:H  | 1:48:A:GLU:H    | 13       | 0.2           |
| (1,556) | 1:47:A:THR:H  | 1:48:A:GLU:H    | 15       | 0.2           |
| (1,556) | 1:47:A:THR:H  | 1:48:A:GLU:H    | 17       | 0.2           |
| (1,556) | 1:47:A:THR:H  | 1:48:A:GLU:H    | 24       | 0.2           |
| (1,556) | 1:47:A:THR:H  | 1:48:A:GLU:H    | 27       | 0.2           |
| (1,556) | 1:47:A:THR:H  | 1:48:A:GLU:H    | 32       | 0.2           |
| (1,556) | 1:47:A:THR:H  | 1:48:A:GLU:H    | 33       | 0.2           |
| (1,556) | 1:47:A:THR:H  | 1:48:A:GLU:H    | 35       | 0.2           |
| (1,556) | 1:47:A:THR:H  | 1:48:A:GLU:H    | 36       | 0.2           |
| (1,549) | 1:71:A:VAL:H  | 1:70:A:ASN:HB2  | 1        | 0.2           |

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| Key     | Atom-1       | Atom-2         | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (1,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2 | 20       | 0.2           |
| (1,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2 | 24       | 0.2           |
| (1,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2 | 33       | 0.2           |
| (1,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2 | 38       | 0.2           |
| (1,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA  | 1        | 0.2           |
| (1,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA  | 8        | 0.2           |
| (1,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA  | 13       | 0.2           |
| (1,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA  | 24       | 0.2           |
| (1,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA  | 38       | 0.2           |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 13       | 0.2           |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2 | 14       | 0.2           |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2 | 28       | 0.2           |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2 | 36       | 0.2           |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H  | 19       | 0.2           |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H  | 20       | 0.2           |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H  | 39       | 0.2           |
| (1,513) | 1:67:A:THR:H | 1:66:A:MET:HG3 | 16       | 0.2           |
| (1,513) | 1:67:A:THR:H | 1:66:A:MET:HG3 | 29       | 0.2           |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2 | 17       | 0.2           |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2 | 38       | 0.2           |
| (1,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2 | 9        | 0.2           |
| (1,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2 | 35       | 0.2           |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA  | 11       | 0.2           |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA  | 14       | 0.2           |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA  | 18       | 0.2           |
| (1,366) | 1:18:A:ASN:H | 1:18:A:ASN:HB3 | 4        | 0.2           |
| (1,366) | 1:18:A:ASN:H | 1:18:A:ASN:HB3 | 11       | 0.2           |
| (1,366) | 1:18:A:ASN:H | 1:18:A:ASN:HB3 | 13       | 0.2           |
| (1,366) | 1:18:A:ASN:H | 1:18:A:ASN:HB3 | 24       | 0.2           |
| (1,366) | 1:18:A:ASN:H | 1:18:A:ASN:HB3 | 25       | 0.2           |
| (1,366) | 1:18:A:ASN:H | 1:18:A:ASN:HB3 | 32       | 0.2           |
| (1,366) | 1:18:A:ASN:H | 1:18:A:ASN:HB3 | 35       | 0.2           |
| (1,366) | 1:18:A:ASN:H | 1:18:A:ASN:HB3 | 36       | 0.2           |
| (1,366) | 1:18:A:ASN:H | 1:18:A:ASN:HB3 | 38       | 0.2           |
| (1,366) | 1:18:A:ASN:H | 1:18:A:ASN:HB3 | 39       | 0.2           |
| (1,366) | 1:18:A:ASN:H | 1:18:A:ASN:HB3 | 40       | 0.2           |
| (1,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA  | 1        | 0.2           |
| (1,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA  | 7        | 0.2           |
| (1,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA  | 8        | 0.2           |
| (1,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA  | 10       | 0.2           |
| (1,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA  | 12       | 0.2           |
| (1,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA  | 31       | 0.2           |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,343) | 1:14:A:LYS:H  | 1:33:A:VAL:HA   | 33       | 0.2           |
| (1,274) | 1:66:A:MET:H  | 1:66:A:MET:HG3  | 28       | 0.2           |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 3        | 0.2           |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 3        | 0.2           |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 3        | 0.2           |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 12       | 0.2           |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 12       | 0.2           |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 12       | 0.2           |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 25       | 0.2           |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 25       | 0.2           |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 25       | 0.2           |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 32       | 0.2           |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 32       | 0.2           |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 32       | 0.2           |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 33       | 0.2           |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 33       | 0.2           |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 33       | 0.2           |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 34       | 0.2           |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 34       | 0.2           |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 34       | 0.2           |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 35       | 0.2           |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 35       | 0.2           |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 35       | 0.2           |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 38       | 0.2           |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 38       | 0.2           |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 38       | 0.2           |
| (1,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 11       | 0.2           |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG21 | 7        | 0.2           |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG22 | 7        | 0.2           |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG23 | 7        | 0.2           |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG21 | 16       | 0.2           |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG22 | 16       | 0.2           |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG23 | 16       | 0.2           |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 1        | 0.2           |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 8        | 0.2           |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 9        | 0.2           |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 31       | 0.2           |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 32       | 0.2           |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 34       | 0.2           |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 35       | 0.2           |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 38       | 0.2           |
| (1,133) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 14       | 0.2           |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,133)  | 1:39:A:ILE:H   | 1:39:A:ILE:HG13 | 16       | 0.2           |
| (1,133)  | 1:39:A:ILE:H   | 1:39:A:ILE:HG13 | 22       | 0.2           |
| (1,133)  | 1:39:A:ILE:H   | 1:39:A:ILE:HG13 | 26       | 0.2           |
| (1,133)  | 1:39:A:ILE:H   | 1:39:A:ILE:HG13 | 32       | 0.2           |
| (1,133)  | 1:39:A:ILE:H   | 1:39:A:ILE:HG13 | 34       | 0.2           |
| (1,100)  | 1:22:A:SER:H   | 1:21:A:VAL:HB   | 39       | 0.2           |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 3        | 0.2           |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 3        | 0.2           |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 3        | 0.2           |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 6        | 0.2           |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 6        | 0.2           |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 6        | 0.2           |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 16       | 0.2           |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 16       | 0.2           |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 16       | 0.2           |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 18       | 0.2           |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 18       | 0.2           |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 18       | 0.2           |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 31       | 0.2           |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 31       | 0.2           |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 31       | 0.2           |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 33       | 0.2           |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 33       | 0.2           |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 33       | 0.2           |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG21 | 40       | 0.2           |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 40       | 0.2           |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 40       | 0.2           |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 1        | 0.19          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 1        | 0.19          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 26       | 0.19          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 26       | 0.19          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 19       | 0.19          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 19       | 0.19          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 28       | 0.19          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 28       | 0.19          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 10       | 0.19          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 10       | 0.19          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 10       | 0.19          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 10       | 0.19          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 10       | 0.19          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 10       | 0.19          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 27       | 0.19          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 27       | 0.19          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 27       | 0.19          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 27       | 0.19          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 27       | 0.19          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 27       | 0.19          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 28       | 0.19          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 28       | 0.19          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 28       | 0.19          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 28       | 0.19          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 28       | 0.19          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 28       | 0.19          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 40       | 0.19          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 40       | 0.19          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 40       | 0.19          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 40       | 0.19          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 40       | 0.19          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 40       | 0.19          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 10       | 0.19          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 10       | 0.19          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 10       | 0.19          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 10       | 0.19          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 6        | 0.19          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 9        | 0.19          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 13       | 0.19          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 16       | 0.19          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 25       | 0.19          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 32       | 0.19          |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2  | 14       | 0.19          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2  | 14       | 0.19          |
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 1        | 0.19          |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 1        | 0.19          |
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 25       | 0.19          |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 25       | 0.19          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 20       | 0.19          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 20       | 0.19          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 28       | 0.19          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 28       | 0.19          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 33       | 0.19          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 33       | 0.19          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 40       | 0.19          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 40       | 0.19          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 20       | 0.19          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 20       | 0.19          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 28       | 0.19          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 28       | 0.19          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 33       | 0.19          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 33       | 0.19          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 40       | 0.19          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 40       | 0.19          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 19       | 0.19          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 1        | 0.19          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 4        | 0.19          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 35       | 0.19          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 4        | 0.19          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 4        | 0.19          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 4        | 0.19          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 18       | 0.19          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 18       | 0.19          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 18       | 0.19          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 23       | 0.19          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 23       | 0.19          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 23       | 0.19          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 40       | 0.19          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 40       | 0.19          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 40       | 0.19          |
| (3,3004) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 18       | 0.19          |
| (3,3004) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 23       | 0.19          |
| (3,3004) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 31       | 0.19          |
| (3,3004) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 32       | 0.19          |
| (3,2938) | 1:26:A:SER:HA  | 1:70:A:ASN:H    | 34       | 0.19          |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 12       | 0.19          |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 19       | 0.19          |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 21       | 0.19          |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 32       | 0.19          |
| (3,2874) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2  | 39       | 0.19          |
| (3,2809) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2  | 4        | 0.19          |
| (3,2809) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2  | 12       | 0.19          |
| (3,2809) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2  | 19       | 0.19          |
| (3,2809) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2  | 21       | 0.19          |
| (3,2809) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2  | 22       | 0.19          |
| (3,2809) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2  | 24       | 0.19          |
| (3,2809) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2  | 27       | 0.19          |
| (3,2809) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2  | 34       | 0.19          |
| (3,2809) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2  | 35       | 0.19          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,2761) | 1:90:A:GLU:HB3 | 1:91:A:ALA:H   | 35       | 0.19          |
| (3,2748) | 1:86:A:GLU:HG3 | 1:87:A:PRO:HA  | 35       | 0.19          |
| (3,2689) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 3        | 0.19          |
| (3,2689) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 6        | 0.19          |
| (3,2689) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 7        | 0.19          |
| (3,2689) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 10       | 0.19          |
| (3,2689) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 11       | 0.19          |
| (3,2689) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 12       | 0.19          |
| (3,2689) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 13       | 0.19          |
| (3,2689) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 15       | 0.19          |
| (3,2689) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 21       | 0.19          |
| (3,2689) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 22       | 0.19          |
| (3,2689) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 24       | 0.19          |
| (3,2689) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 25       | 0.19          |
| (3,2689) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 26       | 0.19          |
| (3,2689) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 28       | 0.19          |
| (3,2689) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 29       | 0.19          |
| (3,2689) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 30       | 0.19          |
| (3,2689) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 31       | 0.19          |
| (3,2689) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 32       | 0.19          |
| (3,2689) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 33       | 0.19          |
| (3,2689) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 34       | 0.19          |
| (3,2689) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 36       | 0.19          |
| (3,2689) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 39       | 0.19          |
| (3,2689) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 40       | 0.19          |
| (3,2680) | 1:53:A:GLN:HA  | 1:53:A:GLN:HB2 | 5        | 0.19          |
| (3,2680) | 1:53:A:GLN:HA  | 1:53:A:GLN:HB2 | 8        | 0.19          |
| (3,2680) | 1:53:A:GLN:HA  | 1:53:A:GLN:HB2 | 9        | 0.19          |
| (3,2680) | 1:53:A:GLN:HA  | 1:53:A:GLN:HB2 | 10       | 0.19          |
| (3,2680) | 1:53:A:GLN:HA  | 1:53:A:GLN:HB2 | 11       | 0.19          |
| (3,2680) | 1:53:A:GLN:HA  | 1:53:A:GLN:HB2 | 15       | 0.19          |
| (3,2680) | 1:53:A:GLN:HA  | 1:53:A:GLN:HB2 | 16       | 0.19          |
| (3,2680) | 1:53:A:GLN:HA  | 1:53:A:GLN:HB2 | 21       | 0.19          |
| (3,2680) | 1:53:A:GLN:HA  | 1:53:A:GLN:HB2 | 23       | 0.19          |
| (3,2680) | 1:53:A:GLN:HA  | 1:53:A:GLN:HB2 | 24       | 0.19          |
| (3,2680) | 1:53:A:GLN:HA  | 1:53:A:GLN:HB2 | 34       | 0.19          |
| (3,2679) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 6        | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 1        | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 2        | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 3        | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 4        | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 5        | 0.19          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 6        | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 7        | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 8        | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 9        | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 10       | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 11       | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 12       | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 13       | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 14       | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 15       | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 16       | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 17       | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 19       | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 20       | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 21       | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 22       | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 23       | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 24       | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 25       | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 26       | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 27       | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 28       | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 29       | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 30       | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 31       | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 32       | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 33       | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 34       | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 35       | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 36       | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 37       | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 38       | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 39       | 0.19          |
| (3,2635) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 40       | 0.19          |
| (3,2617) | 1:74:A:ASP:HB2 | 1:74:A:ASP:HA  | 36       | 0.19          |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 22       | 0.19          |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 39       | 0.19          |
| (3,2554) | 1:92:A:ARG:HA  | 1:83:A:ALA:H   | 24       | 0.19          |
| (3,2554) | 1:92:A:ARG:HA  | 1:83:A:ALA:H   | 25       | 0.19          |
| (3,2554) | 1:92:A:ARG:HA  | 1:83:A:ALA:H   | 30       | 0.19          |
| (3,2554) | 1:92:A:ARG:HA  | 1:83:A:ALA:H   | 39       | 0.19          |
| (3,2538) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 5        | 0.19          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,2538) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 10       | 0.19          |
| (3,2538) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 16       | 0.19          |
| (3,2514) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 11       | 0.19          |
| (3,2514) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 13       | 0.19          |
| (3,2507) | 1:46:A:PRO:HD2 | 1:47:A:THR:HB  | 11       | 0.19          |
| (3,2463) | 1:4:A:PRO:HD3  | 1:3:A:ASP:HA   | 37       | 0.19          |
| (3,2434) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 11       | 0.19          |
| (3,2434) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 35       | 0.19          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 3        | 0.19          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 3        | 0.19          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 3        | 0.19          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 20       | 0.19          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 20       | 0.19          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 20       | 0.19          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 1        | 0.19          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 3        | 0.19          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 10       | 0.19          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 11       | 0.19          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 12       | 0.19          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 13       | 0.19          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 14       | 0.19          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 15       | 0.19          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 17       | 0.19          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 18       | 0.19          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 19       | 0.19          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 21       | 0.19          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 22       | 0.19          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 23       | 0.19          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 24       | 0.19          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 25       | 0.19          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 26       | 0.19          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 27       | 0.19          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 28       | 0.19          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 29       | 0.19          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 30       | 0.19          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 32       | 0.19          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 35       | 0.19          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 36       | 0.19          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 39       | 0.19          |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 4        | 0.19          |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 10       | 0.19          |
| (3,2325) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 16       | 0.19          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 4        | 0.19          |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 12       | 0.19          |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 14       | 0.19          |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 16       | 0.19          |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 27       | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 1        | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 2        | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 3        | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 4        | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 5        | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 6        | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 7        | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 8        | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 10       | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 11       | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 13       | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 15       | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 16       | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 17       | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 18       | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 19       | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 20       | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 21       | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 22       | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 23       | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 24       | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 25       | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 26       | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 27       | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 28       | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 29       | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 30       | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 31       | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 32       | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 33       | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 34       | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 35       | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 36       | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 37       | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 38       | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 39       | 0.19          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 40       | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 8        | 0.19          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 8        | 0.19          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 18       | 0.19          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 18       | 0.19          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 26       | 0.19          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 26       | 0.19          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 29       | 0.19          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 29       | 0.19          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 36       | 0.19          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 36       | 0.19          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 37       | 0.19          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 37       | 0.19          |
| (3,2239) | 1:18:A:ASN:HB3  | 1:18:A:ASN:H    | 12       | 0.19          |
| (3,2218) | 1:56:A:ASN:HA   | 1:56:A:ASN:HD21 | 32       | 0.19          |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 1        | 0.19          |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 6        | 0.19          |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 23       | 0.19          |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 30       | 0.19          |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 33       | 0.19          |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 36       | 0.19          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 11       | 0.19          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 11       | 0.19          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 11       | 0.19          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 14       | 0.19          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 14       | 0.19          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 14       | 0.19          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 23       | 0.19          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 23       | 0.19          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 23       | 0.19          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 26       | 0.19          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 26       | 0.19          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 26       | 0.19          |
| (3,2081) | 1:97:A:LEU:HD11 | 1:21:A:VAL:HB   | 5        | 0.19          |
| (3,2081) | 1:97:A:LEU:HD12 | 1:21:A:VAL:HB   | 5        | 0.19          |
| (3,2081) | 1:97:A:LEU:HD13 | 1:21:A:VAL:HB   | 5        | 0.19          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1  | 37       | 0.19          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2  | 37       | 0.19          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1  | 37       | 0.19          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2  | 37       | 0.19          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1  | 37       | 0.19          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2  | 37       | 0.19          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 7        | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 7        | 0.19          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 7        | 0.19          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 17       | 0.19          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 17       | 0.19          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 17       | 0.19          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 39       | 0.19          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 39       | 0.19          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 39       | 0.19          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1  | 36       | 0.19          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2  | 36       | 0.19          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1  | 36       | 0.19          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2  | 36       | 0.19          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1  | 36       | 0.19          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2  | 36       | 0.19          |
| (3,2019) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD1  | 2        | 0.19          |
| (3,2019) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD2  | 2        | 0.19          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3  | 40       | 0.19          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3  | 40       | 0.19          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3  | 40       | 0.19          |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 1        | 0.19          |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 1        | 0.19          |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 1        | 0.19          |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 14       | 0.19          |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 14       | 0.19          |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 14       | 0.19          |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 34       | 0.19          |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 34       | 0.19          |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 34       | 0.19          |
| (3,1993) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 15       | 0.19          |
| (3,1993) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 15       | 0.19          |
| (3,1993) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 15       | 0.19          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 15       | 0.19          |
| (3,1907) | 1:66:A:MET:HE1  | 1:43:A:TYR:H    | 16       | 0.19          |
| (3,1907) | 1:66:A:MET:HE2  | 1:43:A:TYR:H    | 16       | 0.19          |
| (3,1907) | 1:66:A:MET:HE3  | 1:43:A:TYR:H    | 16       | 0.19          |
| (3,1907) | 1:66:A:MET:HE1  | 1:43:A:TYR:H    | 24       | 0.19          |
| (3,1907) | 1:66:A:MET:HE2  | 1:43:A:TYR:H    | 24       | 0.19          |
| (3,1907) | 1:66:A:MET:HE3  | 1:43:A:TYR:H    | 24       | 0.19          |
| (3,1864) | 1:7:A:ALA:HB1   | 1:88:A:ARG:HA   | 2        | 0.19          |
| (3,1864) | 1:7:A:ALA:HB2   | 1:88:A:ARG:HA   | 2        | 0.19          |
| (3,1864) | 1:7:A:ALA:HB3   | 1:88:A:ARG:HA   | 2        | 0.19          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H    | 35       | 0.19          |

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| Key      | Atom-1           | Atom-2         | Model ID | Violation (Å) |
|----------|------------------|----------------|----------|---------------|
| (3,1856) | 1:27:A:ALA:HB2   | 1:28:A:THR:H   | 35       | 0.19          |
| (3,1856) | 1:27:A:ALA:HB3   | 1:28:A:THR:H   | 35       | 0.19          |
| (3,1856) | 1:27:A:ALA:HB1   | 1:28:A:THR:H   | 37       | 0.19          |
| (3,1856) | 1:27:A:ALA:HB2   | 1:28:A:THR:H   | 37       | 0.19          |
| (3,1856) | 1:27:A:ALA:HB3   | 1:28:A:THR:H   | 37       | 0.19          |
| (3,1856) | 1:27:A:ALA:HB1   | 1:28:A:THR:H   | 38       | 0.19          |
| (3,1856) | 1:27:A:ALA:HB2   | 1:28:A:THR:H   | 38       | 0.19          |
| (3,1856) | 1:27:A:ALA:HB3   | 1:28:A:THR:H   | 38       | 0.19          |
| (3,1856) | 1:27:A:ALA:HB1   | 1:28:A:THR:H   | 40       | 0.19          |
| (3,1856) | 1:27:A:ALA:HB2   | 1:28:A:THR:H   | 40       | 0.19          |
| (3,1856) | 1:27:A:ALA:HB3   | 1:28:A:THR:H   | 40       | 0.19          |
| (3,1828) | 1:98:A:LYS:HD3   | 1:98:A:LYS:HA  | 2        | 0.19          |
| (3,1828) | 1:98:A:LYS:HD3   | 1:98:A:LYS:HA  | 13       | 0.19          |
| (3,1828) | 1:98:A:LYS:HD3   | 1:98:A:LYS:HA  | 15       | 0.19          |
| (3,1828) | 1:98:A:LYS:HD3   | 1:98:A:LYS:HA  | 18       | 0.19          |
| (3,1815) | 1:98:A:LYS:HD3   | 1:98:A:LYS:HA  | 2        | 0.19          |
| (3,1815) | 1:98:A:LYS:HD3   | 1:98:A:LYS:HA  | 13       | 0.19          |
| (3,1815) | 1:98:A:LYS:HD3   | 1:98:A:LYS:HA  | 15       | 0.19          |
| (3,1815) | 1:98:A:LYS:HD3   | 1:98:A:LYS:HA  | 18       | 0.19          |
| (3,1781) | 1:88:A:ARG:HG2   | 1:88:A:ARG:H   | 29       | 0.19          |
| (3,1781) | 1:88:A:ARG:HG2   | 1:88:A:ARG:H   | 38       | 0.19          |
| (3,1747) | 1:51:A:GLU:HG2   | 1:51:A:GLU:H   | 9        | 0.19          |
| (3,1747) | 1:51:A:GLU:HG2   | 1:51:A:GLU:H   | 38       | 0.19          |
| (3,1731) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 4        | 0.19          |
| (3,1731) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 6        | 0.19          |
| (3,1731) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 7        | 0.19          |
| (3,1731) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 10       | 0.19          |
| (3,1731) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 13       | 0.19          |
| (3,1731) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 17       | 0.19          |
| (3,1731) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 21       | 0.19          |
| (3,1731) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 23       | 0.19          |
| (3,1731) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 24       | 0.19          |
| (3,1731) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 25       | 0.19          |
| (3,1731) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 26       | 0.19          |
| (3,1731) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 28       | 0.19          |
| (3,1731) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 30       | 0.19          |
| (3,1731) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 31       | 0.19          |
| (3,1731) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 35       | 0.19          |
| (3,1731) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 36       | 0.19          |
| (3,1731) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 40       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA | 3        | 0.19          |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA | 3        | 0.19          |

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| Key      | Atom-1           | Atom-2         | Model ID | Violation (Å) |
|----------|------------------|----------------|----------|---------------|
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA | 3        | 0.19          |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA | 5        | 0.19          |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA | 5        | 0.19          |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA | 5        | 0.19          |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA | 8        | 0.19          |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA | 8        | 0.19          |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA | 8        | 0.19          |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA | 9        | 0.19          |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA | 9        | 0.19          |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA | 9        | 0.19          |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA | 10       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA | 10       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA | 10       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA | 12       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA | 12       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA | 12       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA | 14       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA | 14       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA | 14       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA | 16       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA | 16       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA | 16       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA | 19       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA | 19       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA | 19       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA | 21       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA | 21       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA | 21       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA | 24       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA | 24       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA | 24       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA | 25       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA | 25       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA | 25       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA | 27       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA | 27       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA | 27       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA | 28       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA | 28       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA | 28       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA | 29       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA | 29       | 0.19          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 29       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 30       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 30       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 30       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 33       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 33       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 33       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 34       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 34       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 34       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 35       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 35       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 35       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 36       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 36       | 0.19          |
| (3,1699) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 36       | 0.19          |
| (3,1682) | 1:85:A:LEU:HD11  | 1:85:A:LEU:HA   | 29       | 0.19          |
| (3,1682) | 1:85:A:LEU:HD12  | 1:85:A:LEU:HA   | 29       | 0.19          |
| (3,1682) | 1:85:A:LEU:HD13  | 1:85:A:LEU:HA   | 29       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG21  | 1:16:A:ILE:HG21 | 17       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG21  | 1:16:A:ILE:HG22 | 17       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG21  | 1:16:A:ILE:HG23 | 17       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG22  | 1:16:A:ILE:HG21 | 17       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG22  | 1:16:A:ILE:HG22 | 17       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG22  | 1:16:A:ILE:HG23 | 17       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG23  | 1:16:A:ILE:HG21 | 17       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG23  | 1:16:A:ILE:HG22 | 17       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG23  | 1:16:A:ILE:HG23 | 17       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG21  | 1:16:A:ILE:HG21 | 19       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG21  | 1:16:A:ILE:HG22 | 19       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG21  | 1:16:A:ILE:HG23 | 19       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG22  | 1:16:A:ILE:HG21 | 19       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG22  | 1:16:A:ILE:HG22 | 19       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG22  | 1:16:A:ILE:HG23 | 19       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG23  | 1:16:A:ILE:HG21 | 19       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG23  | 1:16:A:ILE:HG22 | 19       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG23  | 1:16:A:ILE:HG23 | 19       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG21  | 1:16:A:ILE:HG21 | 29       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG21  | 1:16:A:ILE:HG22 | 29       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG21  | 1:16:A:ILE:HG23 | 29       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG22  | 1:16:A:ILE:HG21 | 29       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG22  | 1:16:A:ILE:HG22 | 29       | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 29       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 29       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 29       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 29       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 36       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 36       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 36       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 36       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 36       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 36       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 36       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 36       | 0.19          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 36       | 0.19          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 12       | 0.19          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 12       | 0.19          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 12       | 0.19          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 16       | 0.19          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 16       | 0.19          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 16       | 0.19          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 29       | 0.19          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 29       | 0.19          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 29       | 0.19          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 33       | 0.19          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 33       | 0.19          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 33       | 0.19          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 37       | 0.19          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 37       | 0.19          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 37       | 0.19          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 16       | 0.19          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 16       | 0.19          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 16       | 0.19          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 24       | 0.19          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 24       | 0.19          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 24       | 0.19          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 27       | 0.19          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 27       | 0.19          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 27       | 0.19          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 34       | 0.19          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 34       | 0.19          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 34       | 0.19          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 38       | 0.19          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 38       | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 38       | 0.19          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 39       | 0.19          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 39       | 0.19          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 39       | 0.19          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 11       | 0.19          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 11       | 0.19          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 11       | 0.19          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 35       | 0.19          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 35       | 0.19          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 35       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 4        | 0.19          |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 4        | 0.19          |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 4        | 0.19          |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 5        | 0.19          |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 5        | 0.19          |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 5        | 0.19          |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 6        | 0.19          |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 6        | 0.19          |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 6        | 0.19          |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 7        | 0.19          |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 7        | 0.19          |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 7        | 0.19          |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 8        | 0.19          |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 8        | 0.19          |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 8        | 0.19          |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 9        | 0.19          |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 9        | 0.19          |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 9        | 0.19          |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 10       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 10       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 10       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 13       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 13       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 13       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 16       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 16       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 16       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 17       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 17       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 17       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 18       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 18       | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 18       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 20       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 20       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 20       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 21       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 21       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 21       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 22       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 22       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 22       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 23       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 23       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 23       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 25       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 25       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 25       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 26       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 26       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 26       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 29       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 29       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 29       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 30       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 30       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 30       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 31       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 31       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 31       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 32       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 32       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 32       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 33       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 33       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 33       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 34       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 34       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 34       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 35       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 35       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 35       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 37       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 37       | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 37       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 38       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 38       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 38       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 39       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 39       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 39       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 40       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 40       | 0.19          |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 40       | 0.19          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 35       | 0.19          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 35       | 0.19          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 35       | 0.19          |
| (3,1534) | 1:2:A:ILE:HG21  | 1:2:A:ILE:HA    | 30       | 0.19          |
| (3,1534) | 1:2:A:ILE:HG22  | 1:2:A:ILE:HA    | 30       | 0.19          |
| (3,1534) | 1:2:A:ILE:HG23  | 1:2:A:ILE:HA    | 30       | 0.19          |
| (3,1534) | 1:2:A:ILE:HG21  | 1:2:A:ILE:HA    | 36       | 0.19          |
| (3,1534) | 1:2:A:ILE:HG22  | 1:2:A:ILE:HA    | 36       | 0.19          |
| (3,1534) | 1:2:A:ILE:HG23  | 1:2:A:ILE:HA    | 36       | 0.19          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1  | 8        | 0.19          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2  | 8        | 0.19          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1  | 8        | 0.19          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2  | 8        | 0.19          |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1  | 8        | 0.19          |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2  | 8        | 0.19          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1  | 11       | 0.19          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2  | 11       | 0.19          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1  | 11       | 0.19          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2  | 11       | 0.19          |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1  | 11       | 0.19          |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2  | 11       | 0.19          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1  | 26       | 0.19          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2  | 26       | 0.19          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1  | 26       | 0.19          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2  | 26       | 0.19          |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1  | 26       | 0.19          |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2  | 26       | 0.19          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1  | 34       | 0.19          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2  | 34       | 0.19          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1  | 34       | 0.19          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2  | 34       | 0.19          |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1  | 34       | 0.19          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2 | 34       | 0.19          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 8        | 0.19          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 8        | 0.19          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 8        | 0.19          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 11       | 0.19          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 11       | 0.19          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 11       | 0.19          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 12       | 0.19          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 12       | 0.19          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 12       | 0.19          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 19       | 0.19          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 19       | 0.19          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 19       | 0.19          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 21       | 0.19          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 21       | 0.19          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 21       | 0.19          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 22       | 0.19          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 22       | 0.19          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 22       | 0.19          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 28       | 0.19          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 28       | 0.19          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 28       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 5        | 0.19          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 5        | 0.19          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 5        | 0.19          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 12       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 12       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 12       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 13       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 13       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 13       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 23       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 23       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 23       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 25       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 25       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 25       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 30       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 30       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 30       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 31       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 31       | 0.19          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 31       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 32       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 32       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 32       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 35       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 35       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 35       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 36       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 36       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 36       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 37       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 37       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 37       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 39       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 39       | 0.19          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 39       | 0.19          |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 5        | 0.19          |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 5        | 0.19          |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 5        | 0.19          |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 18       | 0.19          |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 18       | 0.19          |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 18       | 0.19          |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 27       | 0.19          |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 27       | 0.19          |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 27       | 0.19          |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 29       | 0.19          |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 29       | 0.19          |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 29       | 0.19          |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 31       | 0.19          |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 31       | 0.19          |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 31       | 0.19          |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 36       | 0.19          |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 36       | 0.19          |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 36       | 0.19          |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 37       | 0.19          |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 37       | 0.19          |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 37       | 0.19          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 2        | 0.19          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 2        | 0.19          |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 2        | 0.19          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 3        | 0.19          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 3        | 0.19          |

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| Key      | Atom-1          | Atom-2       | Model ID | Violation (Å) |
|----------|-----------------|--------------|----------|---------------|
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H | 3        | 0.19          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H | 5        | 0.19          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H | 5        | 0.19          |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H | 5        | 0.19          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H | 6        | 0.19          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H | 6        | 0.19          |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H | 6        | 0.19          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H | 11       | 0.19          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H | 11       | 0.19          |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H | 11       | 0.19          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H | 13       | 0.19          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H | 13       | 0.19          |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H | 13       | 0.19          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H | 27       | 0.19          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H | 27       | 0.19          |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H | 27       | 0.19          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H | 32       | 0.19          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H | 32       | 0.19          |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H | 32       | 0.19          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H | 37       | 0.19          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H | 37       | 0.19          |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H | 37       | 0.19          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 9        | 0.19          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 9        | 0.19          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 9        | 0.19          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 15       | 0.19          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 15       | 0.19          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 15       | 0.19          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 33       | 0.19          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 33       | 0.19          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 33       | 0.19          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 35       | 0.19          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 35       | 0.19          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 35       | 0.19          |
| (3,1455) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H | 9        | 0.19          |
| (3,1455) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H | 9        | 0.19          |
| (3,1455) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H | 9        | 0.19          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 2        | 0.19          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 2        | 0.19          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 2        | 0.19          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 4        | 0.19          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 4        | 0.19          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H   | 4        | 0.19          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H   | 6        | 0.19          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H   | 6        | 0.19          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H   | 6        | 0.19          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H   | 20       | 0.19          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H   | 20       | 0.19          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H   | 20       | 0.19          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H   | 29       | 0.19          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H   | 29       | 0.19          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H   | 29       | 0.19          |
| (3,1400) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 7        | 0.19          |
| (3,1400) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 7        | 0.19          |
| (3,1400) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 7        | 0.19          |
| (3,1400) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 11       | 0.19          |
| (3,1400) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 11       | 0.19          |
| (3,1400) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 11       | 0.19          |
| (3,1400) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 21       | 0.19          |
| (3,1400) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 21       | 0.19          |
| (3,1400) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 21       | 0.19          |
| (3,1400) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 24       | 0.19          |
| (3,1400) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 24       | 0.19          |
| (3,1400) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 24       | 0.19          |
| (3,1391) | 1:91:A:ALA:HB1  | 1:12:A:PHE:HZ  | 13       | 0.19          |
| (3,1391) | 1:91:A:ALA:HB2  | 1:12:A:PHE:HZ  | 13       | 0.19          |
| (3,1391) | 1:91:A:ALA:HB3  | 1:12:A:PHE:HZ  | 13       | 0.19          |
| (3,1391) | 1:91:A:ALA:HB1  | 1:12:A:PHE:HZ  | 28       | 0.19          |
| (3,1391) | 1:91:A:ALA:HB2  | 1:12:A:PHE:HZ  | 28       | 0.19          |
| (3,1391) | 1:91:A:ALA:HB3  | 1:12:A:PHE:HZ  | 28       | 0.19          |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3 | 27       | 0.19          |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3 | 36       | 0.19          |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3 | 37       | 0.19          |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 2        | 0.19          |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 2        | 0.19          |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 2        | 0.19          |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 4        | 0.19          |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 4        | 0.19          |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 4        | 0.19          |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 6        | 0.19          |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 6        | 0.19          |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 6        | 0.19          |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 10       | 0.19          |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 10       | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H    | 10       | 0.19          |
| (3,1371) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H    | 16       | 0.19          |
| (3,1371) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H    | 16       | 0.19          |
| (3,1371) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H    | 16       | 0.19          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 13       | 0.19          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 13       | 0.19          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 13       | 0.19          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 15       | 0.19          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 15       | 0.19          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 15       | 0.19          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 22       | 0.19          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 22       | 0.19          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 22       | 0.19          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 28       | 0.19          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 28       | 0.19          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 28       | 0.19          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 29       | 0.19          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 29       | 0.19          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 29       | 0.19          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 31       | 0.19          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 31       | 0.19          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 31       | 0.19          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 32       | 0.19          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 32       | 0.19          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 32       | 0.19          |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 6        | 0.19          |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 6        | 0.19          |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 6        | 0.19          |
| (3,1305) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 16       | 0.19          |
| (3,1305) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 16       | 0.19          |
| (3,1305) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 16       | 0.19          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 2        | 0.19          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 2        | 0.19          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 2        | 0.19          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 7        | 0.19          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 7        | 0.19          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 7        | 0.19          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 2        | 0.19          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 2        | 0.19          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 2        | 0.19          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 7        | 0.19          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 7        | 0.19          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB | 7        | 0.19          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H  | 1        | 0.19          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H  | 1        | 0.19          |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H  | 1        | 0.19          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H  | 2        | 0.19          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H  | 2        | 0.19          |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H  | 2        | 0.19          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H  | 7        | 0.19          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H  | 7        | 0.19          |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H  | 7        | 0.19          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H  | 10       | 0.19          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H  | 10       | 0.19          |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H  | 10       | 0.19          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H  | 14       | 0.19          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H  | 14       | 0.19          |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H  | 14       | 0.19          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H  | 15       | 0.19          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H  | 15       | 0.19          |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H  | 15       | 0.19          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H  | 18       | 0.19          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H  | 18       | 0.19          |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H  | 18       | 0.19          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H  | 21       | 0.19          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H  | 21       | 0.19          |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H  | 21       | 0.19          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H  | 22       | 0.19          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H  | 22       | 0.19          |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H  | 22       | 0.19          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H  | 23       | 0.19          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H  | 23       | 0.19          |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H  | 23       | 0.19          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H  | 24       | 0.19          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H  | 24       | 0.19          |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H  | 24       | 0.19          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H  | 26       | 0.19          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H  | 26       | 0.19          |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H  | 26       | 0.19          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H  | 30       | 0.19          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H  | 30       | 0.19          |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H  | 30       | 0.19          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H  | 36       | 0.19          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H  | 36       | 0.19          |

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| Key      | Atom-1          | Atom-2       | Model ID | Violation (Å) |
|----------|-----------------|--------------|----------|---------------|
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H | 36       | 0.19          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H | 37       | 0.19          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H | 37       | 0.19          |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H | 37       | 0.19          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H | 39       | 0.19          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H | 39       | 0.19          |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H | 39       | 0.19          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H | 1        | 0.19          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H | 1        | 0.19          |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H | 1        | 0.19          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H | 2        | 0.19          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H | 2        | 0.19          |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H | 2        | 0.19          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H | 7        | 0.19          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H | 7        | 0.19          |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H | 7        | 0.19          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H | 10       | 0.19          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H | 10       | 0.19          |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H | 10       | 0.19          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H | 14       | 0.19          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H | 14       | 0.19          |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H | 14       | 0.19          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H | 15       | 0.19          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H | 15       | 0.19          |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H | 15       | 0.19          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H | 18       | 0.19          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H | 18       | 0.19          |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H | 18       | 0.19          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H | 21       | 0.19          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H | 21       | 0.19          |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H | 21       | 0.19          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H | 22       | 0.19          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H | 22       | 0.19          |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H | 22       | 0.19          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H | 23       | 0.19          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H | 23       | 0.19          |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H | 23       | 0.19          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H | 24       | 0.19          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H | 24       | 0.19          |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H | 24       | 0.19          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H | 26       | 0.19          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H | 26       | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 26       | 0.19          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 30       | 0.19          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 30       | 0.19          |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 30       | 0.19          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 36       | 0.19          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 36       | 0.19          |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 36       | 0.19          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 37       | 0.19          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 37       | 0.19          |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 37       | 0.19          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 39       | 0.19          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 39       | 0.19          |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 39       | 0.19          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 7        | 0.19          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 7        | 0.19          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 7        | 0.19          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 21       | 0.19          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 21       | 0.19          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 21       | 0.19          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 24       | 0.19          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 24       | 0.19          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 24       | 0.19          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 29       | 0.19          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 29       | 0.19          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 29       | 0.19          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 32       | 0.19          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 32       | 0.19          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 32       | 0.19          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 33       | 0.19          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 33       | 0.19          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 33       | 0.19          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 39       | 0.19          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 39       | 0.19          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 39       | 0.19          |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 10       | 0.19          |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 15       | 0.19          |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 17       | 0.19          |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 24       | 0.19          |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 40       | 0.19          |
| (3,1181) | 1:100:A:GLU:H   | 1:21:A:VAL:HG11 | 34       | 0.19          |
| (3,1181) | 1:100:A:GLU:H   | 1:21:A:VAL:HG12 | 34       | 0.19          |
| (3,1181) | 1:100:A:GLU:H   | 1:21:A:VAL:HG13 | 34       | 0.19          |

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| Key      | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|----------|---------------|----------------|----------|---------------|
| (3,1173) | 1:14:A:LYS:H  | 1:14:A:LYS:HD2 | 1        | 0.19          |
| (3,1173) | 1:14:A:LYS:H  | 1:14:A:LYS:HD2 | 5        | 0.19          |
| (3,1173) | 1:14:A:LYS:H  | 1:14:A:LYS:HD2 | 17       | 0.19          |
| (3,1173) | 1:14:A:LYS:H  | 1:14:A:LYS:HD2 | 22       | 0.19          |
| (3,1173) | 1:14:A:LYS:H  | 1:14:A:LYS:HD2 | 31       | 0.19          |
| (3,1173) | 1:14:A:LYS:H  | 1:14:A:LYS:HD2 | 34       | 0.19          |
| (3,1173) | 1:14:A:LYS:H  | 1:14:A:LYS:HD2 | 36       | 0.19          |
| (3,1167) | 1:75:A:ASP:H  | 1:74:A:ASP:HB2 | 6        | 0.19          |
| (3,1167) | 1:75:A:ASP:H  | 1:74:A:ASP:HB2 | 12       | 0.19          |
| (3,1167) | 1:75:A:ASP:H  | 1:74:A:ASP:HB2 | 27       | 0.19          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1 | 11       | 0.19          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2 | 11       | 0.19          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1 | 17       | 0.19          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2 | 17       | 0.19          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1 | 19       | 0.19          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2 | 19       | 0.19          |
| (3,1152) | 1:54:A:LYS:H  | 1:53:A:GLN:HG3 | 7        | 0.19          |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 3        | 0.19          |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 10       | 0.19          |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 12       | 0.19          |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 15       | 0.19          |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 17       | 0.19          |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 18       | 0.19          |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 20       | 0.19          |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 23       | 0.19          |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 25       | 0.19          |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 28       | 0.19          |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 30       | 0.19          |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 36       | 0.19          |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 37       | 0.19          |
| (3,1096) | 1:74:A:ASP:H  | 1:73:A:PRO:HA  | 7        | 0.19          |
| (3,1096) | 1:74:A:ASP:H  | 1:73:A:PRO:HA  | 8        | 0.19          |
| (3,1096) | 1:74:A:ASP:H  | 1:73:A:PRO:HA  | 13       | 0.19          |
| (3,1096) | 1:74:A:ASP:H  | 1:73:A:PRO:HA  | 17       | 0.19          |
| (3,1003) | 1:5:A:PHE:H   | 1:4:A:PRO:HA   | 16       | 0.19          |
| (3,942)  | 1:34:A:SER:H  | 1:12:A:PHE:HA  | 40       | 0.19          |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB  | 1        | 0.19          |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB  | 29       | 0.19          |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB  | 33       | 0.19          |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB  | 37       | 0.19          |
| (3,919)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB3 | 22       | 0.19          |
| (3,919)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB3 | 39       | 0.19          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,889) | 1:80:A:SER:H | 1:43:A:TYR:HB3  | 15       | 0.19          |
| (3,889) | 1:80:A:SER:H | 1:43:A:TYR:HB3  | 27       | 0.19          |
| (3,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3   | 23       | 0.19          |
| (3,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3   | 24       | 0.19          |
| (3,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3   | 26       | 0.19          |
| (3,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3   | 27       | 0.19          |
| (3,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3   | 31       | 0.19          |
| (3,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3   | 34       | 0.19          |
| (3,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3   | 38       | 0.19          |
| (3,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3   | 39       | 0.19          |
| (3,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3   | 40       | 0.19          |
| (3,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2   | 3        | 0.19          |
| (3,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2   | 17       | 0.19          |
| (3,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2   | 31       | 0.19          |
| (3,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2   | 34       | 0.19          |
| (3,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2   | 40       | 0.19          |
| (3,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 6        | 0.19          |
| (3,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 13       | 0.19          |
| (3,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 27       | 0.19          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 16       | 0.19          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 16       | 0.19          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 16       | 0.19          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 1        | 0.19          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 1        | 0.19          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 1        | 0.19          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 6        | 0.19          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 6        | 0.19          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 6        | 0.19          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 31       | 0.19          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 31       | 0.19          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 31       | 0.19          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 33       | 0.19          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 33       | 0.19          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 33       | 0.19          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 34       | 0.19          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 34       | 0.19          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 34       | 0.19          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 36       | 0.19          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 36       | 0.19          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 36       | 0.19          |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 5        | 0.19          |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 7        | 0.19          |

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| Key     | Atom-1       | Atom-2         | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2 | 11       | 0.19          |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2 | 13       | 0.19          |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2 | 18       | 0.19          |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2 | 20       | 0.19          |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2 | 23       | 0.19          |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2 | 25       | 0.19          |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2 | 32       | 0.19          |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2 | 37       | 0.19          |
| (3,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2 | 7        | 0.19          |
| (3,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2 | 17       | 0.19          |
| (3,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2 | 26       | 0.19          |
| (3,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2 | 27       | 0.19          |
| (3,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2 | 32       | 0.19          |
| (3,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2 | 36       | 0.19          |
| (3,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA  | 2        | 0.19          |
| (3,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA  | 4        | 0.19          |
| (3,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA  | 8        | 0.19          |
| (3,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA  | 10       | 0.19          |
| (3,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA  | 12       | 0.19          |
| (3,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA  | 13       | 0.19          |
| (3,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA  | 14       | 0.19          |
| (3,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA  | 15       | 0.19          |
| (3,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA  | 16       | 0.19          |
| (3,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA  | 19       | 0.19          |
| (3,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA  | 23       | 0.19          |
| (3,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA  | 24       | 0.19          |
| (3,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA  | 26       | 0.19          |
| (3,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA  | 29       | 0.19          |
| (3,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA  | 30       | 0.19          |
| (3,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA  | 36       | 0.19          |
| (3,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA  | 38       | 0.19          |
| (3,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA  | 39       | 0.19          |
| (3,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 3        | 0.19          |
| (3,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 5        | 0.19          |
| (3,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 25       | 0.19          |
| (3,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 34       | 0.19          |
| (3,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 35       | 0.19          |
| (3,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3 | 2        | 0.19          |
| (3,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3 | 3        | 0.19          |
| (3,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3 | 8        | 0.19          |
| (3,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3 | 9        | 0.19          |
| (3,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3 | 11       | 0.19          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3  | 25       | 0.19          |
| (3,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3  | 30       | 0.19          |
| (3,669) | 1:72:A:THR:H | 1:72:A:THR:HG21 | 18       | 0.19          |
| (3,669) | 1:72:A:THR:H | 1:72:A:THR:HG22 | 18       | 0.19          |
| (3,669) | 1:72:A:THR:H | 1:72:A:THR:HG23 | 18       | 0.19          |
| (3,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2  | 13       | 0.19          |
| (3,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2  | 27       | 0.19          |
| (3,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2  | 31       | 0.19          |
| (3,590) | 1:3:A:ASP:H  | 1:2:A:ILE:HA    | 8        | 0.19          |
| (3,589) | 1:93:A:SER:H | 1:92:A:ARG:HG2  | 21       | 0.19          |
| (3,589) | 1:93:A:SER:H | 1:92:A:ARG:HG2  | 27       | 0.19          |
| (3,589) | 1:93:A:SER:H | 1:92:A:ARG:HG2  | 40       | 0.19          |
| (3,560) | 1:47:A:THR:H | 1:47:A:THR:HA   | 6        | 0.19          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1  | 1        | 0.19          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2  | 1        | 0.19          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1  | 20       | 0.19          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2  | 20       | 0.19          |
| (3,556) | 1:47:A:THR:H | 1:48:A:GLU:H    | 3        | 0.19          |
| (3,556) | 1:47:A:THR:H | 1:48:A:GLU:H    | 9        | 0.19          |
| (3,556) | 1:47:A:THR:H | 1:48:A:GLU:H    | 14       | 0.19          |
| (3,556) | 1:47:A:THR:H | 1:48:A:GLU:H    | 20       | 0.19          |
| (3,556) | 1:47:A:THR:H | 1:48:A:GLU:H    | 21       | 0.19          |
| (3,556) | 1:47:A:THR:H | 1:48:A:GLU:H    | 22       | 0.19          |
| (3,556) | 1:47:A:THR:H | 1:48:A:GLU:H    | 23       | 0.19          |
| (3,556) | 1:47:A:THR:H | 1:48:A:GLU:H    | 25       | 0.19          |
| (3,556) | 1:47:A:THR:H | 1:48:A:GLU:H    | 30       | 0.19          |
| (3,556) | 1:47:A:THR:H | 1:48:A:GLU:H    | 34       | 0.19          |
| (3,556) | 1:47:A:THR:H | 1:48:A:GLU:H    | 40       | 0.19          |
| (3,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 12       | 0.19          |
| (3,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 23       | 0.19          |
| (3,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 16       | 0.19          |
| (3,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 21       | 0.19          |
| (3,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 25       | 0.19          |
| (3,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 27       | 0.19          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 18       | 0.19          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 7        | 0.19          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 19       | 0.19          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 1        | 0.19          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 3        | 0.19          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 8        | 0.19          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 10       | 0.19          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 12       | 0.19          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 27       | 0.19          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 28       | 0.19          |
| (3,513) | 1:67:A:THR:H | 1:66:A:MET:HG3  | 28       | 0.19          |
| (3,513) | 1:67:A:THR:H | 1:66:A:MET:HG3  | 39       | 0.19          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 26       | 0.19          |
| (3,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 7        | 0.19          |
| (3,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2  | 27       | 0.19          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 13       | 0.19          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 19       | 0.19          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 27       | 0.19          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 35       | 0.19          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 37       | 0.19          |
| (3,366) | 1:18:A:ASN:H | 1:18:A:ASN:HB3  | 12       | 0.19          |
| (3,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 6        | 0.19          |
| (3,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 14       | 0.19          |
| (3,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 24       | 0.19          |
| (3,274) | 1:66:A:MET:H | 1:66:A:MET:HG3  | 2        | 0.19          |
| (3,274) | 1:66:A:MET:H | 1:66:A:MET:HG3  | 12       | 0.19          |
| (3,274) | 1:66:A:MET:H | 1:66:A:MET:HG3  | 19       | 0.19          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 1        | 0.19          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 1        | 0.19          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 1        | 0.19          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 2        | 0.19          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 2        | 0.19          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 2        | 0.19          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 7        | 0.19          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 7        | 0.19          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 7        | 0.19          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 10       | 0.19          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 10       | 0.19          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 10       | 0.19          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 14       | 0.19          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 14       | 0.19          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 14       | 0.19          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 15       | 0.19          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 15       | 0.19          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 15       | 0.19          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 18       | 0.19          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 18       | 0.19          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 18       | 0.19          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 21       | 0.19          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 21       | 0.19          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 21       | 0.19          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 22       | 0.19          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 22       | 0.19          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 22       | 0.19          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 23       | 0.19          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 23       | 0.19          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 23       | 0.19          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 24       | 0.19          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 24       | 0.19          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 24       | 0.19          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 26       | 0.19          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 26       | 0.19          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 26       | 0.19          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 30       | 0.19          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 30       | 0.19          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 30       | 0.19          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 36       | 0.19          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 36       | 0.19          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 36       | 0.19          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 37       | 0.19          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 37       | 0.19          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 37       | 0.19          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 39       | 0.19          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 39       | 0.19          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 39       | 0.19          |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 13       | 0.19          |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 23       | 0.19          |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 29       | 0.19          |
| (3,176) | 1:10:A:ILE:H  | 1:35:A:PHE:HD1  | 31       | 0.19          |
| (3,176) | 1:10:A:ILE:H  | 1:35:A:PHE:HD2  | 31       | 0.19          |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 3        | 0.19          |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 10       | 0.19          |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 12       | 0.19          |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 15       | 0.19          |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 17       | 0.19          |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 18       | 0.19          |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 20       | 0.19          |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 23       | 0.19          |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 25       | 0.19          |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 28       | 0.19          |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 30       | 0.19          |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 36       | 0.19          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 37       | 0.19          |
| (3,135) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 1        | 0.19          |
| (3,135) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 3        | 0.19          |
| (3,135) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 15       | 0.19          |
| (3,135) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 18       | 0.19          |
| (3,135) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 20       | 0.19          |
| (3,135) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 23       | 0.19          |
| (3,135) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 25       | 0.19          |
| (3,135) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 27       | 0.19          |
| (3,135) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 28       | 0.19          |
| (3,135) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 29       | 0.19          |
| (3,135) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 30       | 0.19          |
| (3,135) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 31       | 0.19          |
| (3,135) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 33       | 0.19          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 4        | 0.19          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 12       | 0.19          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 19       | 0.19          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 20       | 0.19          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 31       | 0.19          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 32       | 0.19          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 35       | 0.19          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 38       | 0.19          |
| (3,74)  | 1:51:A:GLU:H  | 1:50:A:THR:HG21 | 10       | 0.19          |
| (3,74)  | 1:51:A:GLU:H  | 1:50:A:THR:HG22 | 10       | 0.19          |
| (3,74)  | 1:51:A:GLU:H  | 1:50:A:THR:HG23 | 10       | 0.19          |
| (3,74)  | 1:51:A:GLU:H  | 1:50:A:THR:HG21 | 19       | 0.19          |
| (3,74)  | 1:51:A:GLU:H  | 1:50:A:THR:HG22 | 19       | 0.19          |
| (3,74)  | 1:51:A:GLU:H  | 1:50:A:THR:HG23 | 19       | 0.19          |
| (3,74)  | 1:51:A:GLU:H  | 1:50:A:THR:HG21 | 37       | 0.19          |
| (3,74)  | 1:51:A:GLU:H  | 1:50:A:THR:HG22 | 37       | 0.19          |
| (3,74)  | 1:51:A:GLU:H  | 1:50:A:THR:HG23 | 37       | 0.19          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 9        | 0.19          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 38       | 0.19          |
| (3,59)  | 1:42:A:TRP:H  | 1:41:A:THR:HB   | 31       | 0.19          |
| (3,51)  | 1:57:A:PHE:H  | 1:56:A:ASN:HB2  | 3        | 0.19          |
| (3,51)  | 1:57:A:PHE:H  | 1:56:A:ASN:HB2  | 8        | 0.19          |
| (3,51)  | 1:57:A:PHE:H  | 1:56:A:ASN:HB2  | 15       | 0.19          |
| (3,51)  | 1:57:A:PHE:H  | 1:56:A:ASN:HB2  | 24       | 0.19          |
| (3,51)  | 1:57:A:PHE:H  | 1:56:A:ASN:HB2  | 27       | 0.19          |
| (3,51)  | 1:57:A:PHE:H  | 1:56:A:ASN:HB2  | 28       | 0.19          |
| (3,51)  | 1:57:A:PHE:H  | 1:56:A:ASN:HB2  | 30       | 0.19          |
| (3,51)  | 1:57:A:PHE:H  | 1:56:A:ASN:HB2  | 31       | 0.19          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 1        | 0.19          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 1        | 0.19          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 26       | 0.19          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 26       | 0.19          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 19       | 0.19          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 19       | 0.19          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 28       | 0.19          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 28       | 0.19          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 10       | 0.19          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 10       | 0.19          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 10       | 0.19          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 10       | 0.19          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 10       | 0.19          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 10       | 0.19          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 27       | 0.19          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 27       | 0.19          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 27       | 0.19          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 27       | 0.19          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 27       | 0.19          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 27       | 0.19          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 28       | 0.19          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 28       | 0.19          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 28       | 0.19          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 28       | 0.19          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 28       | 0.19          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 28       | 0.19          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 40       | 0.19          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 40       | 0.19          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 40       | 0.19          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 40       | 0.19          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 40       | 0.19          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 40       | 0.19          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 10       | 0.19          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 10       | 0.19          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 10       | 0.19          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 10       | 0.19          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 6        | 0.19          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 9        | 0.19          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 13       | 0.19          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 16       | 0.19          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 25       | 0.19          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 32       | 0.19          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2  | 14       | 0.19          |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2  | 14       | 0.19          |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 1        | 0.19          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 1        | 0.19          |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 25       | 0.19          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 25       | 0.19          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 20       | 0.19          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 20       | 0.19          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 28       | 0.19          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 28       | 0.19          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 33       | 0.19          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 33       | 0.19          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 40       | 0.19          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 40       | 0.19          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 20       | 0.19          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 20       | 0.19          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 28       | 0.19          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 28       | 0.19          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 33       | 0.19          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 33       | 0.19          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 40       | 0.19          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 40       | 0.19          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 19       | 0.19          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 1        | 0.19          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 4        | 0.19          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 35       | 0.19          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 4        | 0.19          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 4        | 0.19          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 4        | 0.19          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 18       | 0.19          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 18       | 0.19          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 18       | 0.19          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 23       | 0.19          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 23       | 0.19          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 23       | 0.19          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 40       | 0.19          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 40       | 0.19          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 40       | 0.19          |
| (1,2996) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 18       | 0.19          |
| (1,2996) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 23       | 0.19          |
| (1,2996) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 31       | 0.19          |
| (1,2996) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 32       | 0.19          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,2931) | 1:26:A:SER:HA  | 1:70:A:ASN:H   | 34       | 0.19          |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2 | 12       | 0.19          |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2 | 19       | 0.19          |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2 | 21       | 0.19          |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2 | 32       | 0.19          |
| (1,2867) | 1:92:A:ARG:HD2 | 1:92:A:ARG:HG2 | 39       | 0.19          |
| (1,2802) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2 | 4        | 0.19          |
| (1,2802) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2 | 12       | 0.19          |
| (1,2802) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2 | 19       | 0.19          |
| (1,2802) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2 | 21       | 0.19          |
| (1,2802) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2 | 22       | 0.19          |
| (1,2802) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2 | 24       | 0.19          |
| (1,2802) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2 | 27       | 0.19          |
| (1,2802) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2 | 34       | 0.19          |
| (1,2802) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2 | 35       | 0.19          |
| (1,2754) | 1:90:A:GLU:HB3 | 1:91:A:ALA:H   | 35       | 0.19          |
| (1,2685) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 3        | 0.19          |
| (1,2685) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 6        | 0.19          |
| (1,2685) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 7        | 0.19          |
| (1,2685) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 10       | 0.19          |
| (1,2685) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 11       | 0.19          |
| (1,2685) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 12       | 0.19          |
| (1,2685) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 13       | 0.19          |
| (1,2685) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 15       | 0.19          |
| (1,2685) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 21       | 0.19          |
| (1,2685) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 22       | 0.19          |
| (1,2685) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 24       | 0.19          |
| (1,2685) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 25       | 0.19          |
| (1,2685) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 26       | 0.19          |
| (1,2685) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 28       | 0.19          |
| (1,2685) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 29       | 0.19          |
| (1,2685) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 30       | 0.19          |
| (1,2685) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 31       | 0.19          |
| (1,2685) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 32       | 0.19          |
| (1,2685) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 33       | 0.19          |
| (1,2685) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 34       | 0.19          |
| (1,2685) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 36       | 0.19          |
| (1,2685) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 39       | 0.19          |
| (1,2685) | 1:8:A:GLU:HB2  | 1:8:A:GLU:HG2  | 40       | 0.19          |
| (1,2676) | 1:53:A:GLN:HA  | 1:53:A:GLN:HB2 | 5        | 0.19          |
| (1,2676) | 1:53:A:GLN:HA  | 1:53:A:GLN:HB2 | 8        | 0.19          |
| (1,2676) | 1:53:A:GLN:HA  | 1:53:A:GLN:HB2 | 9        | 0.19          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,2676) | 1:53:A:GLN:HA  | 1:53:A:GLN:HB2 | 10       | 0.19          |
| (1,2676) | 1:53:A:GLN:HA  | 1:53:A:GLN:HB2 | 11       | 0.19          |
| (1,2676) | 1:53:A:GLN:HA  | 1:53:A:GLN:HB2 | 15       | 0.19          |
| (1,2676) | 1:53:A:GLN:HA  | 1:53:A:GLN:HB2 | 16       | 0.19          |
| (1,2676) | 1:53:A:GLN:HA  | 1:53:A:GLN:HB2 | 21       | 0.19          |
| (1,2676) | 1:53:A:GLN:HA  | 1:53:A:GLN:HB2 | 23       | 0.19          |
| (1,2676) | 1:53:A:GLN:HA  | 1:53:A:GLN:HB2 | 24       | 0.19          |
| (1,2676) | 1:53:A:GLN:HA  | 1:53:A:GLN:HB2 | 34       | 0.19          |
| (1,2675) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 6        | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 1        | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 2        | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 3        | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 4        | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 5        | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 6        | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 7        | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 8        | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 9        | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 10       | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 11       | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 12       | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 13       | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 14       | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 15       | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 16       | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 17       | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 19       | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 20       | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 21       | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 22       | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 23       | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 24       | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 25       | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 26       | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 27       | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 28       | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 29       | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 30       | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 31       | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 32       | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 33       | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 34       | 0.19          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 35       | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 36       | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 37       | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 38       | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 39       | 0.19          |
| (1,2631) | 1:11:A:GLN:HB3 | 1:11:A:GLN:HG3 | 40       | 0.19          |
| (1,2613) | 1:74:A:ASP:HB2 | 1:74:A:ASP:HA  | 36       | 0.19          |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 22       | 0.19          |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 39       | 0.19          |
| (1,2550) | 1:92:A:ARG:HA  | 1:83:A:ALA:H   | 24       | 0.19          |
| (1,2550) | 1:92:A:ARG:HA  | 1:83:A:ALA:H   | 25       | 0.19          |
| (1,2550) | 1:92:A:ARG:HA  | 1:83:A:ALA:H   | 30       | 0.19          |
| (1,2550) | 1:92:A:ARG:HA  | 1:83:A:ALA:H   | 39       | 0.19          |
| (1,2534) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 5        | 0.19          |
| (1,2534) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 10       | 0.19          |
| (1,2534) | 1:73:A:PRO:HD3 | 1:73:A:PRO:HB3 | 16       | 0.19          |
| (1,2511) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 11       | 0.19          |
| (1,2511) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 13       | 0.19          |
| (1,2460) | 1:4:A:PRO:HD3  | 1:3:A:ASP:HA   | 37       | 0.19          |
| (1,2431) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 11       | 0.19          |
| (1,2431) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 35       | 0.19          |
| (1,2402) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 3        | 0.19          |
| (1,2402) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 3        | 0.19          |
| (1,2402) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 3        | 0.19          |
| (1,2402) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 20       | 0.19          |
| (1,2402) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 20       | 0.19          |
| (1,2402) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 20       | 0.19          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 1        | 0.19          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 3        | 0.19          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 10       | 0.19          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 11       | 0.19          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 12       | 0.19          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 13       | 0.19          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 14       | 0.19          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 15       | 0.19          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 17       | 0.19          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 18       | 0.19          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 19       | 0.19          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 21       | 0.19          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 22       | 0.19          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 23       | 0.19          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 24       | 0.19          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 25       | 0.19          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 26       | 0.19          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 27       | 0.19          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 28       | 0.19          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 29       | 0.19          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 30       | 0.19          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 32       | 0.19          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 35       | 0.19          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 36       | 0.19          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 39       | 0.19          |
| (1,2322) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 4        | 0.19          |
| (1,2322) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 10       | 0.19          |
| (1,2322) | 1:80:A:SER:HB2 | 1:81:A:VAL:H   | 16       | 0.19          |
| (1,2286) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 4        | 0.19          |
| (1,2286) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 12       | 0.19          |
| (1,2286) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 14       | 0.19          |
| (1,2286) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 16       | 0.19          |
| (1,2286) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 27       | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 1        | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 2        | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 3        | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 4        | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 5        | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 6        | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 7        | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 8        | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 10       | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 11       | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 13       | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 15       | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 16       | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 17       | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 18       | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 19       | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 20       | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 21       | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 22       | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 23       | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 24       | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 25       | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 26       | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 27       | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2278) | 1:96:A:GLU:HG3  | 1:96:A:GLU:HB3  | 28       | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3  | 1:96:A:GLU:HB3  | 29       | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3  | 1:96:A:GLU:HB3  | 30       | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3  | 1:96:A:GLU:HB3  | 31       | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3  | 1:96:A:GLU:HB3  | 32       | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3  | 1:96:A:GLU:HB3  | 33       | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3  | 1:96:A:GLU:HB3  | 34       | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3  | 1:96:A:GLU:HB3  | 35       | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3  | 1:96:A:GLU:HB3  | 36       | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3  | 1:96:A:GLU:HB3  | 37       | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3  | 1:96:A:GLU:HB3  | 38       | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3  | 1:96:A:GLU:HB3  | 39       | 0.19          |
| (1,2278) | 1:96:A:GLU:HG3  | 1:96:A:GLU:HB3  | 40       | 0.19          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 8        | 0.19          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 8        | 0.19          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 18       | 0.19          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 18       | 0.19          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 26       | 0.19          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 26       | 0.19          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 29       | 0.19          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 29       | 0.19          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 36       | 0.19          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 36       | 0.19          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 37       | 0.19          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 37       | 0.19          |
| (1,2236) | 1:18:A:ASN:HB3  | 1:18:A:ASN:H    | 12       | 0.19          |
| (1,2215) | 1:56:A:ASN:HA   | 1:56:A:ASN:HD21 | 32       | 0.19          |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 1        | 0.19          |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 6        | 0.19          |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 23       | 0.19          |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 30       | 0.19          |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 33       | 0.19          |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 36       | 0.19          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 11       | 0.19          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 11       | 0.19          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 11       | 0.19          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 14       | 0.19          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 14       | 0.19          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 14       | 0.19          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 23       | 0.19          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 23       | 0.19          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 23       | 0.19          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2 | 26       | 0.19          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2 | 26       | 0.19          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2 | 26       | 0.19          |
| (1,2076) | 1:97:A:LEU:HD11 | 1:21:A:VAL:HB  | 5        | 0.19          |
| (1,2076) | 1:97:A:LEU:HD12 | 1:21:A:VAL:HB  | 5        | 0.19          |
| (1,2076) | 1:97:A:LEU:HD13 | 1:21:A:VAL:HB  | 5        | 0.19          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 16       | 0.19          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 16       | 0.19          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 16       | 0.19          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 37       | 0.19          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 37       | 0.19          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 37       | 0.19          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 37       | 0.19          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 37       | 0.19          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 37       | 0.19          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 7        | 0.19          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 7        | 0.19          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 7        | 0.19          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 17       | 0.19          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 17       | 0.19          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 17       | 0.19          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 39       | 0.19          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 39       | 0.19          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 39       | 0.19          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 36       | 0.19          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 36       | 0.19          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 36       | 0.19          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 36       | 0.19          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 36       | 0.19          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 36       | 0.19          |
| (1,2014) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD1 | 2        | 0.19          |
| (1,2014) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD2 | 2        | 0.19          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3 | 40       | 0.19          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3 | 40       | 0.19          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3 | 40       | 0.19          |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2 | 1        | 0.19          |
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2 | 1        | 0.19          |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2 | 1        | 0.19          |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2 | 14       | 0.19          |
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2 | 14       | 0.19          |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2 | 14       | 0.19          |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2 | 34       | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 34       | 0.19          |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 34       | 0.19          |
| (1,1990) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 15       | 0.19          |
| (1,1990) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 15       | 0.19          |
| (1,1990) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 15       | 0.19          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 15       | 0.19          |
| (1,1904) | 1:66:A:MET:HE1  | 1:43:A:TYR:H    | 16       | 0.19          |
| (1,1904) | 1:66:A:MET:HE2  | 1:43:A:TYR:H    | 16       | 0.19          |
| (1,1904) | 1:66:A:MET:HE3  | 1:43:A:TYR:H    | 16       | 0.19          |
| (1,1904) | 1:66:A:MET:HE1  | 1:43:A:TYR:H    | 24       | 0.19          |
| (1,1904) | 1:66:A:MET:HE2  | 1:43:A:TYR:H    | 24       | 0.19          |
| (1,1904) | 1:66:A:MET:HE3  | 1:43:A:TYR:H    | 24       | 0.19          |
| (1,1861) | 1:7:A:ALA:HB1   | 1:88:A:ARG:HA   | 2        | 0.19          |
| (1,1861) | 1:7:A:ALA:HB2   | 1:88:A:ARG:HA   | 2        | 0.19          |
| (1,1861) | 1:7:A:ALA:HB3   | 1:88:A:ARG:HA   | 2        | 0.19          |
| (1,1853) | 1:27:A:ALA:HB1  | 1:28:A:THR:H    | 35       | 0.19          |
| (1,1853) | 1:27:A:ALA:HB2  | 1:28:A:THR:H    | 35       | 0.19          |
| (1,1853) | 1:27:A:ALA:HB3  | 1:28:A:THR:H    | 35       | 0.19          |
| (1,1853) | 1:27:A:ALA:HB1  | 1:28:A:THR:H    | 37       | 0.19          |
| (1,1853) | 1:27:A:ALA:HB2  | 1:28:A:THR:H    | 37       | 0.19          |
| (1,1853) | 1:27:A:ALA:HB3  | 1:28:A:THR:H    | 37       | 0.19          |
| (1,1853) | 1:27:A:ALA:HB1  | 1:28:A:THR:H    | 38       | 0.19          |
| (1,1853) | 1:27:A:ALA:HB2  | 1:28:A:THR:H    | 38       | 0.19          |
| (1,1853) | 1:27:A:ALA:HB3  | 1:28:A:THR:H    | 38       | 0.19          |
| (1,1853) | 1:27:A:ALA:HB1  | 1:28:A:THR:H    | 40       | 0.19          |
| (1,1853) | 1:27:A:ALA:HB2  | 1:28:A:THR:H    | 40       | 0.19          |
| (1,1853) | 1:27:A:ALA:HB3  | 1:28:A:THR:H    | 40       | 0.19          |
| (1,1825) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 2        | 0.19          |
| (1,1825) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 13       | 0.19          |
| (1,1825) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 15       | 0.19          |
| (1,1825) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 18       | 0.19          |
| (1,1812) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 2        | 0.19          |
| (1,1812) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 13       | 0.19          |
| (1,1812) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 15       | 0.19          |
| (1,1812) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 18       | 0.19          |
| (1,1778) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H    | 29       | 0.19          |
| (1,1778) | 1:88:A:ARG:HG2  | 1:88:A:ARG:H    | 38       | 0.19          |
| (1,1744) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 9        | 0.19          |
| (1,1744) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 38       | 0.19          |
| (1,1728) | 1:48:A:GLU:HB2  | 1:48:A:GLU:H    | 4        | 0.19          |
| (1,1728) | 1:48:A:GLU:HB2  | 1:48:A:GLU:H    | 6        | 0.19          |
| (1,1728) | 1:48:A:GLU:HB2  | 1:48:A:GLU:H    | 7        | 0.19          |

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| Key      | Atom-1           | Atom-2         | Model ID | Violation (Å) |
|----------|------------------|----------------|----------|---------------|
| (1,1728) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 10       | 0.19          |
| (1,1728) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 13       | 0.19          |
| (1,1728) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 17       | 0.19          |
| (1,1728) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 21       | 0.19          |
| (1,1728) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 23       | 0.19          |
| (1,1728) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 24       | 0.19          |
| (1,1728) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 25       | 0.19          |
| (1,1728) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 26       | 0.19          |
| (1,1728) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 28       | 0.19          |
| (1,1728) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 30       | 0.19          |
| (1,1728) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 31       | 0.19          |
| (1,1728) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 35       | 0.19          |
| (1,1728) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 36       | 0.19          |
| (1,1728) | 1:48:A:GLU:HB2   | 1:48:A:GLU:H   | 40       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA | 3        | 0.19          |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA | 3        | 0.19          |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA | 3        | 0.19          |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA | 5        | 0.19          |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA | 5        | 0.19          |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA | 5        | 0.19          |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA | 8        | 0.19          |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA | 8        | 0.19          |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA | 8        | 0.19          |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA | 9        | 0.19          |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA | 9        | 0.19          |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA | 9        | 0.19          |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA | 10       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA | 10       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA | 10       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA | 12       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA | 12       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA | 12       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA | 14       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA | 14       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA | 14       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA | 16       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA | 16       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA | 16       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA | 19       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA | 19       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA | 19       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA | 21       | 0.19          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 21       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 21       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 24       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 24       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 24       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 25       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 25       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 25       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 27       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 27       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 27       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 28       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 28       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 28       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 29       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 29       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 29       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 30       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 30       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 30       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 33       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 33       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 33       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 34       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 34       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 34       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 35       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 35       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 35       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD11 | 1:101:A:LEU:HA  | 36       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD12 | 1:101:A:LEU:HA  | 36       | 0.19          |
| (1,1695) | 1:101:A:LEU:HD13 | 1:101:A:LEU:HA  | 36       | 0.19          |
| (1,1678) | 1:85:A:LEU:HD11  | 1:85:A:LEU:HA   | 29       | 0.19          |
| (1,1678) | 1:85:A:LEU:HD12  | 1:85:A:LEU:HA   | 29       | 0.19          |
| (1,1678) | 1:85:A:LEU:HD13  | 1:85:A:LEU:HA   | 29       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG21  | 1:16:A:ILE:HG21 | 17       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG21  | 1:16:A:ILE:HG22 | 17       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG21  | 1:16:A:ILE:HG23 | 17       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG22  | 1:16:A:ILE:HG21 | 17       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG22  | 1:16:A:ILE:HG22 | 17       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG22  | 1:16:A:ILE:HG23 | 17       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG23  | 1:16:A:ILE:HG21 | 17       | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 17       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 17       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 19       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 19       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 19       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 19       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 19       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 19       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 19       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 19       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 19       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 29       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 29       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 29       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 29       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 29       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 29       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 29       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 29       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 29       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 36       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 36       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 36       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 36       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 36       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 36       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 36       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 36       | 0.19          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 36       | 0.19          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 12       | 0.19          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 12       | 0.19          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 12       | 0.19          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 16       | 0.19          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 16       | 0.19          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 16       | 0.19          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 29       | 0.19          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 29       | 0.19          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 29       | 0.19          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 33       | 0.19          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 33       | 0.19          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 33       | 0.19          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 37       | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 37       | 0.19          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 37       | 0.19          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 16       | 0.19          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 16       | 0.19          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 16       | 0.19          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 24       | 0.19          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 24       | 0.19          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 24       | 0.19          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 27       | 0.19          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 27       | 0.19          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 27       | 0.19          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 34       | 0.19          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 34       | 0.19          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 34       | 0.19          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 38       | 0.19          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 38       | 0.19          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 38       | 0.19          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 39       | 0.19          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 39       | 0.19          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 39       | 0.19          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 11       | 0.19          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 11       | 0.19          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 11       | 0.19          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 35       | 0.19          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 35       | 0.19          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 35       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 4        | 0.19          |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 4        | 0.19          |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 4        | 0.19          |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 5        | 0.19          |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 5        | 0.19          |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 5        | 0.19          |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 6        | 0.19          |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 6        | 0.19          |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 6        | 0.19          |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 7        | 0.19          |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 7        | 0.19          |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 7        | 0.19          |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 8        | 0.19          |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 8        | 0.19          |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 8        | 0.19          |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 9        | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 9        | 0.19          |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 9        | 0.19          |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 10       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 10       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 10       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 13       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 13       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 13       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 16       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 16       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 16       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 17       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 17       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 17       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 18       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 18       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 18       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 20       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 20       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 20       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 21       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 21       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 21       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 22       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 22       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 22       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 23       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 23       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 23       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 25       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 25       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 25       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 26       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 26       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 26       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 29       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 29       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 29       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 30       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 30       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 30       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 31       | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 31       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 31       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 32       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 32       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 32       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 33       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 33       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 33       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 34       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 34       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 34       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 35       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 35       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 35       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 37       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 37       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 37       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 38       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 38       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 38       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 39       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 39       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 39       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 40       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 40       | 0.19          |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 40       | 0.19          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 35       | 0.19          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 35       | 0.19          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 35       | 0.19          |
| (1,1530) | 1:2:A:ILE:HG21  | 1:2:A:ILE:HA    | 30       | 0.19          |
| (1,1530) | 1:2:A:ILE:HG22  | 1:2:A:ILE:HA    | 30       | 0.19          |
| (1,1530) | 1:2:A:ILE:HG23  | 1:2:A:ILE:HA    | 30       | 0.19          |
| (1,1530) | 1:2:A:ILE:HG21  | 1:2:A:ILE:HA    | 36       | 0.19          |
| (1,1530) | 1:2:A:ILE:HG22  | 1:2:A:ILE:HA    | 36       | 0.19          |
| (1,1530) | 1:2:A:ILE:HG23  | 1:2:A:ILE:HA    | 36       | 0.19          |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1  | 8        | 0.19          |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2  | 8        | 0.19          |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1  | 8        | 0.19          |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2  | 8        | 0.19          |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1  | 8        | 0.19          |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2  | 8        | 0.19          |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1  | 11       | 0.19          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2 | 11       | 0.19          |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1 | 11       | 0.19          |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2 | 11       | 0.19          |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1 | 11       | 0.19          |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2 | 11       | 0.19          |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1 | 26       | 0.19          |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2 | 26       | 0.19          |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1 | 26       | 0.19          |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2 | 26       | 0.19          |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1 | 26       | 0.19          |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2 | 26       | 0.19          |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1 | 34       | 0.19          |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2 | 34       | 0.19          |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1 | 34       | 0.19          |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2 | 34       | 0.19          |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1 | 34       | 0.19          |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2 | 34       | 0.19          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 8        | 0.19          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 8        | 0.19          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 8        | 0.19          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 11       | 0.19          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 11       | 0.19          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 11       | 0.19          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 12       | 0.19          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 12       | 0.19          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 12       | 0.19          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 19       | 0.19          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 19       | 0.19          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 19       | 0.19          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 21       | 0.19          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 21       | 0.19          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 21       | 0.19          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 22       | 0.19          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 22       | 0.19          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 22       | 0.19          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 28       | 0.19          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 28       | 0.19          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 28       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 5        | 0.19          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 5        | 0.19          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 5        | 0.19          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 12       | 0.19          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 12       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 12       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 13       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 13       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 13       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 23       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 23       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 23       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 25       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 25       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 25       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 30       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 30       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 30       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 31       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 31       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 31       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 32       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 32       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 32       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 35       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 35       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 35       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 36       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 36       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 36       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 37       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 37       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 37       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 39       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 39       | 0.19          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 39       | 0.19          |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 5        | 0.19          |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 5        | 0.19          |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 5        | 0.19          |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 18       | 0.19          |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 18       | 0.19          |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 18       | 0.19          |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 27       | 0.19          |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 27       | 0.19          |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 27       | 0.19          |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 29       | 0.19          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 29       | 0.19          |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 29       | 0.19          |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 31       | 0.19          |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 31       | 0.19          |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 31       | 0.19          |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 36       | 0.19          |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 36       | 0.19          |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 36       | 0.19          |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 37       | 0.19          |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 37       | 0.19          |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 37       | 0.19          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 2        | 0.19          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 2        | 0.19          |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 2        | 0.19          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 3        | 0.19          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 3        | 0.19          |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 3        | 0.19          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 5        | 0.19          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 5        | 0.19          |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 5        | 0.19          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 6        | 0.19          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 6        | 0.19          |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 6        | 0.19          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 11       | 0.19          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 11       | 0.19          |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 11       | 0.19          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 13       | 0.19          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 13       | 0.19          |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 13       | 0.19          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 27       | 0.19          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 27       | 0.19          |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 27       | 0.19          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 32       | 0.19          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 32       | 0.19          |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 32       | 0.19          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 37       | 0.19          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 37       | 0.19          |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 37       | 0.19          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H   | 9        | 0.19          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H   | 9        | 0.19          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H   | 9        | 0.19          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H   | 15       | 0.19          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H  | 15       | 0.19          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H  | 15       | 0.19          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H  | 33       | 0.19          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H  | 33       | 0.19          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H  | 33       | 0.19          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H  | 35       | 0.19          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H  | 35       | 0.19          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H  | 35       | 0.19          |
| (1,1451) | 1:71:A:VAL:HG11 | 1:71:A:VAL:H  | 9        | 0.19          |
| (1,1451) | 1:71:A:VAL:HG12 | 1:71:A:VAL:H  | 9        | 0.19          |
| (1,1451) | 1:71:A:VAL:HG13 | 1:71:A:VAL:H  | 9        | 0.19          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H  | 2        | 0.19          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H  | 2        | 0.19          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H  | 2        | 0.19          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H  | 4        | 0.19          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H  | 4        | 0.19          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H  | 4        | 0.19          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H  | 6        | 0.19          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H  | 6        | 0.19          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H  | 6        | 0.19          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H  | 20       | 0.19          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H  | 20       | 0.19          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H  | 20       | 0.19          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H  | 29       | 0.19          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H  | 29       | 0.19          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H  | 29       | 0.19          |
| (1,1396) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA | 7        | 0.19          |
| (1,1396) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA | 7        | 0.19          |
| (1,1396) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA | 7        | 0.19          |
| (1,1396) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA | 11       | 0.19          |
| (1,1396) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA | 11       | 0.19          |
| (1,1396) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA | 11       | 0.19          |
| (1,1396) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA | 21       | 0.19          |
| (1,1396) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA | 21       | 0.19          |
| (1,1396) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA | 21       | 0.19          |
| (1,1396) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA | 24       | 0.19          |
| (1,1396) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA | 24       | 0.19          |
| (1,1396) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA | 24       | 0.19          |
| (1,1387) | 1:91:A:ALA:HB1  | 1:12:A:PHE:HZ | 13       | 0.19          |
| (1,1387) | 1:91:A:ALA:HB2  | 1:12:A:PHE:HZ | 13       | 0.19          |
| (1,1387) | 1:91:A:ALA:HB3  | 1:12:A:PHE:HZ | 13       | 0.19          |
| (1,1387) | 1:91:A:ALA:HB1  | 1:12:A:PHE:HZ | 28       | 0.19          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1387) | 1:91:A:ALA:HB2  | 1:12:A:PHE:HZ  | 28       | 0.19          |
| (1,1387) | 1:91:A:ALA:HB3  | 1:12:A:PHE:HZ  | 28       | 0.19          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3 | 27       | 0.19          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3 | 36       | 0.19          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3 | 37       | 0.19          |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 2        | 0.19          |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 2        | 0.19          |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 2        | 0.19          |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 4        | 0.19          |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 4        | 0.19          |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 4        | 0.19          |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 6        | 0.19          |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 6        | 0.19          |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 6        | 0.19          |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 10       | 0.19          |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 10       | 0.19          |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 10       | 0.19          |
| (1,1367) | 1:16:A:ILE:HG21 | 1:17:A:GLN:H   | 16       | 0.19          |
| (1,1367) | 1:16:A:ILE:HG22 | 1:17:A:GLN:H   | 16       | 0.19          |
| (1,1367) | 1:16:A:ILE:HG23 | 1:17:A:GLN:H   | 16       | 0.19          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 13       | 0.19          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 13       | 0.19          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 13       | 0.19          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 15       | 0.19          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 15       | 0.19          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 15       | 0.19          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 22       | 0.19          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 22       | 0.19          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 22       | 0.19          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 28       | 0.19          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 28       | 0.19          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 28       | 0.19          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 29       | 0.19          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 29       | 0.19          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 29       | 0.19          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 31       | 0.19          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 31       | 0.19          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 31       | 0.19          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2 | 32       | 0.19          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2 | 32       | 0.19          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2 | 32       | 0.19          |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA  | 6        | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 6        | 0.19          |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 6        | 0.19          |
| (1,1301) | 1:19:A:ILE:HD11 | 1:19:A:ILE:HA   | 16       | 0.19          |
| (1,1301) | 1:19:A:ILE:HD12 | 1:19:A:ILE:HA   | 16       | 0.19          |
| (1,1301) | 1:19:A:ILE:HD13 | 1:19:A:ILE:HA   | 16       | 0.19          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 2        | 0.19          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 2        | 0.19          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 2        | 0.19          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 7        | 0.19          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 7        | 0.19          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 7        | 0.19          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 2        | 0.19          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 2        | 0.19          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 2        | 0.19          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 7        | 0.19          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 7        | 0.19          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 7        | 0.19          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 1        | 0.19          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 1        | 0.19          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 1        | 0.19          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 2        | 0.19          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 2        | 0.19          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 2        | 0.19          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 7        | 0.19          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 7        | 0.19          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 7        | 0.19          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 10       | 0.19          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 10       | 0.19          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 10       | 0.19          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 14       | 0.19          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 14       | 0.19          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 14       | 0.19          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 15       | 0.19          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 15       | 0.19          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 15       | 0.19          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 18       | 0.19          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 18       | 0.19          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 18       | 0.19          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 21       | 0.19          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 21       | 0.19          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 21       | 0.19          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 22       | 0.19          |

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| Key      | Atom-1          | Atom-2       | Model ID | Violation (Å) |
|----------|-----------------|--------------|----------|---------------|
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H | 22       | 0.19          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H | 22       | 0.19          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H | 23       | 0.19          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H | 23       | 0.19          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H | 23       | 0.19          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H | 24       | 0.19          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H | 24       | 0.19          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H | 24       | 0.19          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H | 26       | 0.19          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H | 26       | 0.19          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H | 26       | 0.19          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H | 30       | 0.19          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H | 30       | 0.19          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H | 30       | 0.19          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H | 36       | 0.19          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H | 36       | 0.19          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H | 36       | 0.19          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H | 37       | 0.19          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H | 37       | 0.19          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H | 37       | 0.19          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H | 39       | 0.19          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H | 39       | 0.19          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H | 39       | 0.19          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H | 1        | 0.19          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H | 1        | 0.19          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H | 1        | 0.19          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H | 2        | 0.19          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H | 2        | 0.19          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H | 2        | 0.19          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H | 7        | 0.19          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H | 7        | 0.19          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H | 7        | 0.19          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H | 10       | 0.19          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H | 10       | 0.19          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H | 10       | 0.19          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H | 14       | 0.19          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H | 14       | 0.19          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H | 14       | 0.19          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H | 15       | 0.19          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H | 15       | 0.19          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H | 15       | 0.19          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H | 18       | 0.19          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 18       | 0.19          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 18       | 0.19          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 21       | 0.19          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 21       | 0.19          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 21       | 0.19          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 22       | 0.19          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 22       | 0.19          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 22       | 0.19          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 23       | 0.19          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 23       | 0.19          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 23       | 0.19          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 24       | 0.19          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 24       | 0.19          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 24       | 0.19          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 26       | 0.19          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 26       | 0.19          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 26       | 0.19          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 30       | 0.19          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 30       | 0.19          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 30       | 0.19          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 36       | 0.19          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 36       | 0.19          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 36       | 0.19          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 37       | 0.19          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 37       | 0.19          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 37       | 0.19          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 39       | 0.19          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 39       | 0.19          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 39       | 0.19          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3 | 7        | 0.19          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3 | 7        | 0.19          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3 | 7        | 0.19          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3 | 21       | 0.19          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3 | 21       | 0.19          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3 | 21       | 0.19          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3 | 24       | 0.19          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3 | 24       | 0.19          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3 | 24       | 0.19          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3 | 29       | 0.19          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3 | 29       | 0.19          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3 | 29       | 0.19          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3 | 32       | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 32       | 0.19          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 32       | 0.19          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 33       | 0.19          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 33       | 0.19          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 33       | 0.19          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 39       | 0.19          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 39       | 0.19          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 39       | 0.19          |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 10       | 0.19          |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 15       | 0.19          |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 17       | 0.19          |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 24       | 0.19          |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 40       | 0.19          |
| (1,1177) | 1:100:A:GLU:H   | 1:21:A:VAL:HG11 | 34       | 0.19          |
| (1,1177) | 1:100:A:GLU:H   | 1:21:A:VAL:HG12 | 34       | 0.19          |
| (1,1177) | 1:100:A:GLU:H   | 1:21:A:VAL:HG13 | 34       | 0.19          |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 1        | 0.19          |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 5        | 0.19          |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 17       | 0.19          |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 22       | 0.19          |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 31       | 0.19          |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 34       | 0.19          |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 36       | 0.19          |
| (1,1163) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 6        | 0.19          |
| (1,1163) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 12       | 0.19          |
| (1,1163) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 27       | 0.19          |
| (1,1162) | 1:97:A:LEU:H    | 1:29:A:PHE:HE1  | 11       | 0.19          |
| (1,1162) | 1:97:A:LEU:H    | 1:29:A:PHE:HE2  | 11       | 0.19          |
| (1,1162) | 1:97:A:LEU:H    | 1:29:A:PHE:HE1  | 17       | 0.19          |
| (1,1162) | 1:97:A:LEU:H    | 1:29:A:PHE:HE2  | 17       | 0.19          |
| (1,1162) | 1:97:A:LEU:H    | 1:29:A:PHE:HE1  | 19       | 0.19          |
| (1,1162) | 1:97:A:LEU:H    | 1:29:A:PHE:HE2  | 19       | 0.19          |
| (1,1149) | 1:54:A:LYS:H    | 1:53:A:GLN:HG3  | 7        | 0.19          |
| (1,1137) | 1:100:A:GLU:H   | 1:101:A:LEU:H   | 3        | 0.19          |
| (1,1137) | 1:100:A:GLU:H   | 1:101:A:LEU:H   | 10       | 0.19          |
| (1,1137) | 1:100:A:GLU:H   | 1:101:A:LEU:H   | 12       | 0.19          |
| (1,1137) | 1:100:A:GLU:H   | 1:101:A:LEU:H   | 15       | 0.19          |
| (1,1137) | 1:100:A:GLU:H   | 1:101:A:LEU:H   | 17       | 0.19          |
| (1,1137) | 1:100:A:GLU:H   | 1:101:A:LEU:H   | 18       | 0.19          |
| (1,1137) | 1:100:A:GLU:H   | 1:101:A:LEU:H   | 20       | 0.19          |
| (1,1137) | 1:100:A:GLU:H   | 1:101:A:LEU:H   | 23       | 0.19          |
| (1,1137) | 1:100:A:GLU:H   | 1:101:A:LEU:H   | 25       | 0.19          |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 28       | 0.19          |
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 30       | 0.19          |
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 36       | 0.19          |
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 37       | 0.19          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 7        | 0.19          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 8        | 0.19          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 13       | 0.19          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 17       | 0.19          |
| (1,1002) | 1:5:A:PHE:H   | 1:4:A:PRO:HA    | 16       | 0.19          |
| (1,941)  | 1:34:A:SER:H  | 1:12:A:PHE:HA   | 40       | 0.19          |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 1        | 0.19          |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 29       | 0.19          |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 33       | 0.19          |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 37       | 0.19          |
| (1,918)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB3  | 22       | 0.19          |
| (1,918)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB3  | 39       | 0.19          |
| (1,888)  | 1:80:A:SER:H  | 1:43:A:TYR:HB3  | 15       | 0.19          |
| (1,888)  | 1:80:A:SER:H  | 1:43:A:TYR:HB3  | 27       | 0.19          |
| (1,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3   | 23       | 0.19          |
| (1,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3   | 24       | 0.19          |
| (1,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3   | 26       | 0.19          |
| (1,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3   | 27       | 0.19          |
| (1,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3   | 31       | 0.19          |
| (1,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3   | 34       | 0.19          |
| (1,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3   | 38       | 0.19          |
| (1,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3   | 39       | 0.19          |
| (1,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3   | 40       | 0.19          |
| (1,870)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD2   | 3        | 0.19          |
| (1,870)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD2   | 17       | 0.19          |
| (1,870)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD2   | 31       | 0.19          |
| (1,870)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD2   | 34       | 0.19          |
| (1,870)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD2   | 40       | 0.19          |
| (1,869)  | 1:8:A:GLU:H   | 1:7:A:ALA:HA    | 6        | 0.19          |
| (1,869)  | 1:8:A:GLU:H   | 1:7:A:ALA:HA    | 13       | 0.19          |
| (1,869)  | 1:8:A:GLU:H   | 1:7:A:ALA:HA    | 27       | 0.19          |
| (1,849)  | 1:83:A:ALA:H  | 1:91:A:ALA:HB1  | 16       | 0.19          |
| (1,849)  | 1:83:A:ALA:H  | 1:91:A:ALA:HB2  | 16       | 0.19          |
| (1,849)  | 1:83:A:ALA:H  | 1:91:A:ALA:HB3  | 16       | 0.19          |
| (1,814)  | 1:25:A:GLN:H  | 1:71:A:VAL:HG21 | 1        | 0.19          |
| (1,814)  | 1:25:A:GLN:H  | 1:71:A:VAL:HG22 | 1        | 0.19          |
| (1,814)  | 1:25:A:GLN:H  | 1:71:A:VAL:HG23 | 1        | 0.19          |
| (1,814)  | 1:25:A:GLN:H  | 1:71:A:VAL:HG21 | 6        | 0.19          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 6        | 0.19          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 6        | 0.19          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 31       | 0.19          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 31       | 0.19          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 31       | 0.19          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 33       | 0.19          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 33       | 0.19          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 33       | 0.19          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 34       | 0.19          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 34       | 0.19          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 34       | 0.19          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 36       | 0.19          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 36       | 0.19          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 36       | 0.19          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 5        | 0.19          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 7        | 0.19          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 11       | 0.19          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 13       | 0.19          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 18       | 0.19          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 20       | 0.19          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 23       | 0.19          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 25       | 0.19          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 32       | 0.19          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 37       | 0.19          |
| (1,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2  | 7        | 0.19          |
| (1,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2  | 17       | 0.19          |
| (1,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2  | 26       | 0.19          |
| (1,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2  | 27       | 0.19          |
| (1,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2  | 32       | 0.19          |
| (1,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2  | 36       | 0.19          |
| (1,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 2        | 0.19          |
| (1,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 4        | 0.19          |
| (1,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 8        | 0.19          |
| (1,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 10       | 0.19          |
| (1,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 12       | 0.19          |
| (1,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 13       | 0.19          |
| (1,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 14       | 0.19          |
| (1,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 15       | 0.19          |
| (1,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 16       | 0.19          |
| (1,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 19       | 0.19          |
| (1,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 23       | 0.19          |
| (1,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 24       | 0.19          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 26       | 0.19          |
| (1,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 29       | 0.19          |
| (1,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 30       | 0.19          |
| (1,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 36       | 0.19          |
| (1,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 38       | 0.19          |
| (1,737) | 1:15:A:ARG:H | 1:14:A:LYS:HA   | 39       | 0.19          |
| (1,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2  | 3        | 0.19          |
| (1,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2  | 5        | 0.19          |
| (1,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2  | 25       | 0.19          |
| (1,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2  | 34       | 0.19          |
| (1,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2  | 35       | 0.19          |
| (1,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3  | 2        | 0.19          |
| (1,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3  | 3        | 0.19          |
| (1,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3  | 8        | 0.19          |
| (1,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3  | 9        | 0.19          |
| (1,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3  | 11       | 0.19          |
| (1,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3  | 25       | 0.19          |
| (1,715) | 1:16:A:ILE:H | 1:15:A:ARG:HB3  | 30       | 0.19          |
| (1,669) | 1:72:A:THR:H | 1:72:A:THR:HG21 | 18       | 0.19          |
| (1,669) | 1:72:A:THR:H | 1:72:A:THR:HG22 | 18       | 0.19          |
| (1,669) | 1:72:A:THR:H | 1:72:A:THR:HG23 | 18       | 0.19          |
| (1,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2  | 13       | 0.19          |
| (1,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2  | 27       | 0.19          |
| (1,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2  | 31       | 0.19          |
| (1,590) | 1:3:A:ASP:H  | 1:2:A:ILE:HA    | 8        | 0.19          |
| (1,560) | 1:47:A:THR:H | 1:47:A:THR:HA   | 6        | 0.19          |
| (1,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1  | 1        | 0.19          |
| (1,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2  | 1        | 0.19          |
| (1,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1  | 20       | 0.19          |
| (1,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2  | 20       | 0.19          |
| (1,556) | 1:47:A:THR:H | 1:48:A:GLU:H    | 3        | 0.19          |
| (1,556) | 1:47:A:THR:H | 1:48:A:GLU:H    | 9        | 0.19          |
| (1,556) | 1:47:A:THR:H | 1:48:A:GLU:H    | 14       | 0.19          |
| (1,556) | 1:47:A:THR:H | 1:48:A:GLU:H    | 20       | 0.19          |
| (1,556) | 1:47:A:THR:H | 1:48:A:GLU:H    | 21       | 0.19          |
| (1,556) | 1:47:A:THR:H | 1:48:A:GLU:H    | 22       | 0.19          |
| (1,556) | 1:47:A:THR:H | 1:48:A:GLU:H    | 23       | 0.19          |
| (1,556) | 1:47:A:THR:H | 1:48:A:GLU:H    | 25       | 0.19          |
| (1,556) | 1:47:A:THR:H | 1:48:A:GLU:H    | 30       | 0.19          |
| (1,556) | 1:47:A:THR:H | 1:48:A:GLU:H    | 34       | 0.19          |
| (1,556) | 1:47:A:THR:H | 1:48:A:GLU:H    | 40       | 0.19          |
| (1,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 12       | 0.19          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 23       | 0.19          |
| (1,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 16       | 0.19          |
| (1,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 21       | 0.19          |
| (1,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 25       | 0.19          |
| (1,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 27       | 0.19          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 18       | 0.19          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 7        | 0.19          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 19       | 0.19          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 1        | 0.19          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 3        | 0.19          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 8        | 0.19          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 10       | 0.19          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 12       | 0.19          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 27       | 0.19          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 28       | 0.19          |
| (1,513) | 1:67:A:THR:H | 1:66:A:MET:HG3  | 28       | 0.19          |
| (1,513) | 1:67:A:THR:H | 1:66:A:MET:HG3  | 39       | 0.19          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 26       | 0.19          |
| (1,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 7        | 0.19          |
| (1,423) | 1:69:A:HIS:H | 1:69:A:HIS:HD2  | 27       | 0.19          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 13       | 0.19          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 19       | 0.19          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 27       | 0.19          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 35       | 0.19          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 37       | 0.19          |
| (1,366) | 1:18:A:ASN:H | 1:18:A:ASN:HB3  | 12       | 0.19          |
| (1,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 6        | 0.19          |
| (1,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 14       | 0.19          |
| (1,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 24       | 0.19          |
| (1,274) | 1:66:A:MET:H | 1:66:A:MET:HG3  | 2        | 0.19          |
| (1,274) | 1:66:A:MET:H | 1:66:A:MET:HG3  | 12       | 0.19          |
| (1,274) | 1:66:A:MET:H | 1:66:A:MET:HG3  | 19       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 1        | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 1        | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 1        | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 2        | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 2        | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 2        | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 7        | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 7        | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 7        | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 10       | 0.19          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 10       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 10       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 14       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 14       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 14       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 15       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 15       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 15       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 18       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 18       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 18       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 21       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 21       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 21       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 22       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 22       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 22       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 23       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 23       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 23       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 24       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 24       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 24       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 26       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 26       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 26       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 30       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 30       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 30       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 36       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 36       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 36       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 37       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 37       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 37       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 39       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 39       | 0.19          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 39       | 0.19          |
| (1,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 13       | 0.19          |
| (1,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 23       | 0.19          |
| (1,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 29       | 0.19          |
| (1,176) | 1:10:A:ILE:H | 1:35:A:PHE:HD1  | 31       | 0.19          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,176) | 1:10:A:ILE:H  | 1:35:A:PHE:HD2  | 31       | 0.19          |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 3        | 0.19          |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 10       | 0.19          |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 12       | 0.19          |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 15       | 0.19          |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 17       | 0.19          |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 18       | 0.19          |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 20       | 0.19          |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 23       | 0.19          |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 25       | 0.19          |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 28       | 0.19          |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 30       | 0.19          |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 36       | 0.19          |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 37       | 0.19          |
| (1,133) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 1        | 0.19          |
| (1,133) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 3        | 0.19          |
| (1,133) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 15       | 0.19          |
| (1,133) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 18       | 0.19          |
| (1,133) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 20       | 0.19          |
| (1,133) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 23       | 0.19          |
| (1,133) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 25       | 0.19          |
| (1,133) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 27       | 0.19          |
| (1,133) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 28       | 0.19          |
| (1,133) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 29       | 0.19          |
| (1,133) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 30       | 0.19          |
| (1,133) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 31       | 0.19          |
| (1,133) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 33       | 0.19          |
| (1,100) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 4        | 0.19          |
| (1,100) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 12       | 0.19          |
| (1,100) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 19       | 0.19          |
| (1,100) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 20       | 0.19          |
| (1,100) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 31       | 0.19          |
| (1,100) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 32       | 0.19          |
| (1,100) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 35       | 0.19          |
| (1,100) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 38       | 0.19          |
| (1,72)  | 1:51:A:GLU:H  | 1:50:A:THR:HG21 | 10       | 0.19          |
| (1,72)  | 1:51:A:GLU:H  | 1:50:A:THR:HG22 | 10       | 0.19          |
| (1,72)  | 1:51:A:GLU:H  | 1:50:A:THR:HG23 | 10       | 0.19          |
| (1,72)  | 1:51:A:GLU:H  | 1:50:A:THR:HG21 | 19       | 0.19          |
| (1,72)  | 1:51:A:GLU:H  | 1:50:A:THR:HG22 | 19       | 0.19          |
| (1,72)  | 1:51:A:GLU:H  | 1:50:A:THR:HG23 | 19       | 0.19          |
| (1,72)  | 1:51:A:GLU:H  | 1:50:A:THR:HG21 | 37       | 0.19          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG22 | 37       | 0.19          |
| (1,72)   | 1:51:A:GLU:H   | 1:50:A:THR:HG23 | 37       | 0.19          |
| (1,70)   | 1:51:A:GLU:H   | 1:51:A:GLU:HG2  | 9        | 0.19          |
| (1,70)   | 1:51:A:GLU:H   | 1:51:A:GLU:HG2  | 38       | 0.19          |
| (1,57)   | 1:42:A:TRP:H   | 1:41:A:THR:HB   | 31       | 0.19          |
| (1,49)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2  | 3        | 0.19          |
| (1,49)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2  | 8        | 0.19          |
| (1,49)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2  | 15       | 0.19          |
| (1,49)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2  | 24       | 0.19          |
| (1,49)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2  | 27       | 0.19          |
| (1,49)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2  | 28       | 0.19          |
| (1,49)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2  | 30       | 0.19          |
| (1,49)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2  | 31       | 0.19          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 7        | 0.18          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 7        | 0.18          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 14       | 0.18          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 14       | 0.18          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 34       | 0.18          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 34       | 0.18          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 12       | 0.18          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 12       | 0.18          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 12       | 0.18          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 12       | 0.18          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 12       | 0.18          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 12       | 0.18          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 16       | 0.18          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 16       | 0.18          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 16       | 0.18          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 16       | 0.18          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 16       | 0.18          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 16       | 0.18          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 24       | 0.18          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 24       | 0.18          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 24       | 0.18          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 24       | 0.18          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 24       | 0.18          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 24       | 0.18          |
| (3,3205) | 1:43:A:TYR:HD1 | 1:80:A:SER:HB2  | 34       | 0.18          |
| (3,3205) | 1:43:A:TYR:HD2 | 1:80:A:SER:HB2  | 34       | 0.18          |
| (3,3205) | 1:43:A:TYR:HD1 | 1:80:A:SER:HB2  | 37       | 0.18          |
| (3,3205) | 1:43:A:TYR:HD2 | 1:80:A:SER:HB2  | 37       | 0.18          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 6        | 0.18          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2 | 6        | 0.18          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1 | 6        | 0.18          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2 | 6        | 0.18          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1 | 12       | 0.18          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2 | 12       | 0.18          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1 | 12       | 0.18          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2 | 12       | 0.18          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB  | 3        | 0.18          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB  | 12       | 0.18          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB  | 23       | 0.18          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB  | 27       | 0.18          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB  | 28       | 0.18          |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 9        | 0.18          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 9        | 0.18          |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 15       | 0.18          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 15       | 0.18          |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 29       | 0.18          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 29       | 0.18          |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 39       | 0.18          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 39       | 0.18          |
| (3,3138) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB2 | 20       | 0.18          |
| (3,3138) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB2 | 20       | 0.18          |
| (3,3137) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3 | 22       | 0.18          |
| (3,3137) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3 | 22       | 0.18          |
| (3,3137) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3 | 25       | 0.18          |
| (3,3137) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3 | 25       | 0.18          |
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2 | 31       | 0.18          |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2 | 31       | 0.18          |
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2 | 32       | 0.18          |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2 | 32       | 0.18          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 5        | 0.18          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 5        | 0.18          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 10       | 0.18          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 10       | 0.18          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 21       | 0.18          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 21       | 0.18          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 24       | 0.18          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 24       | 0.18          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 31       | 0.18          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 31       | 0.18          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 34       | 0.18          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 34       | 0.18          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 5        | 0.18          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 5        | 0.18          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 10       | 0.18          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 10       | 0.18          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 21       | 0.18          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 21       | 0.18          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 24       | 0.18          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 24       | 0.18          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 31       | 0.18          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 31       | 0.18          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 34       | 0.18          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 34       | 0.18          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 1        | 0.18          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 1        | 0.18          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 1        | 0.18          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 1        | 0.18          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 1        | 0.18          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 1        | 0.18          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 36       | 0.18          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 36       | 0.18          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 36       | 0.18          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 36       | 0.18          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 36       | 0.18          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 36       | 0.18          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 6        | 0.18          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 6        | 0.18          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 6        | 0.18          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 6        | 0.18          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 6        | 0.18          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 6        | 0.18          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 17       | 0.18          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 17       | 0.18          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 17       | 0.18          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 17       | 0.18          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 17       | 0.18          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 17       | 0.18          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 28       | 0.18          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 28       | 0.18          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 28       | 0.18          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 28       | 0.18          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 28       | 0.18          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 28       | 0.18          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 7        | 0.18          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 8        | 0.18          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 12       | 0.18          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 16       | 0.18          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 18       | 0.18          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 20       | 0.18          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 3        | 0.18          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 3        | 0.18          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 3        | 0.18          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 17       | 0.18          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 17       | 0.18          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 17       | 0.18          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 5        | 0.18          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 5        | 0.18          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 8        | 0.18          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 8        | 0.18          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 5        | 0.18          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 7        | 0.18          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 8        | 0.18          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 11       | 0.18          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 19       | 0.18          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 26       | 0.18          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 32       | 0.18          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 36       | 0.18          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 40       | 0.18          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 7        | 0.18          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 7        | 0.18          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 7        | 0.18          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 10       | 0.18          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 10       | 0.18          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 10       | 0.18          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 16       | 0.18          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 16       | 0.18          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 16       | 0.18          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 21       | 0.18          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 21       | 0.18          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 21       | 0.18          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 25       | 0.18          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 25       | 0.18          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 25       | 0.18          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 28       | 0.18          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 28       | 0.18          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 28       | 0.18          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 31       | 0.18          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 31       | 0.18          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 31       | 0.18          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 32       | 0.18          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 32       | 0.18          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 32       | 0.18          |
| (3,3004) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 13       | 0.18          |
| (3,3004) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 19       | 0.18          |
| (3,2938) | 1:26:A:SER:HA  | 1:70:A:ASN:H    | 1        | 0.18          |
| (3,2938) | 1:26:A:SER:HA  | 1:70:A:ASN:H    | 18       | 0.18          |
| (3,2938) | 1:26:A:SER:HA  | 1:70:A:ASN:H    | 39       | 0.18          |
| (3,2925) | 1:22:A:SER:HB2 | 1:25:A:GLN:H    | 15       | 0.18          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 3        | 0.18          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 5        | 0.18          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 6        | 0.18          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 7        | 0.18          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 8        | 0.18          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 14       | 0.18          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 15       | 0.18          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 16       | 0.18          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 17       | 0.18          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 19       | 0.18          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 24       | 0.18          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 26       | 0.18          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 35       | 0.18          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 37       | 0.18          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 40       | 0.18          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3  | 3        | 0.18          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3  | 5        | 0.18          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3  | 6        | 0.18          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3  | 7        | 0.18          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3  | 8        | 0.18          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3  | 14       | 0.18          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3  | 15       | 0.18          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3  | 16       | 0.18          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3  | 17       | 0.18          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3  | 19       | 0.18          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3  | 24       | 0.18          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3  | 26       | 0.18          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3  | 35       | 0.18          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3  | 37       | 0.18          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2911) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HE3 | 40       | 0.18          |
| (3,2809) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HB2 | 17       | 0.18          |
| (3,2809) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HB2 | 26       | 0.18          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H  | 2        | 0.18          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H  | 22       | 0.18          |
| (3,2761) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H   | 26       | 0.18          |
| (3,2748) | 1:86:A:GLU:HG3  | 1:87:A:PRO:HA  | 29       | 0.18          |
| (3,2690) | 1:8:A:GLU:HB3   | 1:8:A:GLU:HG2  | 2        | 0.18          |
| (3,2689) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 1        | 0.18          |
| (3,2689) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 2        | 0.18          |
| (3,2689) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 4        | 0.18          |
| (3,2689) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 5        | 0.18          |
| (3,2689) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 8        | 0.18          |
| (3,2689) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 9        | 0.18          |
| (3,2689) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 14       | 0.18          |
| (3,2689) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 17       | 0.18          |
| (3,2689) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 18       | 0.18          |
| (3,2689) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 19       | 0.18          |
| (3,2689) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 20       | 0.18          |
| (3,2689) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 23       | 0.18          |
| (3,2689) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 27       | 0.18          |
| (3,2689) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 35       | 0.18          |
| (3,2689) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 37       | 0.18          |
| (3,2689) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 38       | 0.18          |
| (3,2679) | 1:25:A:GLN:HG3  | 1:26:A:SER:H   | 26       | 0.18          |
| (3,2635) | 1:11:A:GLN:HB3  | 1:11:A:GLN:HG3 | 18       | 0.18          |
| (3,2619) | 1:74:A:ASP:HB3  | 1:74:A:ASP:H   | 36       | 0.18          |
| (3,2601) | 1:36:A:ASP:HB3  | 1:37:A:ASP:H   | 24       | 0.18          |
| (3,2601) | 1:36:A:ASP:HB3  | 1:37:A:ASP:H   | 38       | 0.18          |
| (3,2554) | 1:92:A:ARG:HA   | 1:83:A:ALA:H   | 17       | 0.18          |
| (3,2554) | 1:92:A:ARG:HA   | 1:83:A:ALA:H   | 21       | 0.18          |
| (3,2541) | 1:73:A:PRO:HG3  | 1:73:A:PRO:HA  | 31       | 0.18          |
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 1        | 0.18          |
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 2        | 0.18          |
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 3        | 0.18          |
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 4        | 0.18          |
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 5        | 0.18          |
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 6        | 0.18          |
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 8        | 0.18          |
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 15       | 0.18          |
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 18       | 0.18          |
| (3,2514) | 1:46:A:PRO:HB3  | 1:46:A:PRO:HD2 | 20       | 0.18          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,2463) | 1:4:A:PRO:HD3  | 1:3:A:ASP:HA   | 6        | 0.18          |
| (3,2463) | 1:4:A:PRO:HD3  | 1:3:A:ASP:HA   | 22       | 0.18          |
| (3,2434) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 1        | 0.18          |
| (3,2434) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 13       | 0.18          |
| (3,2412) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 8        | 0.18          |
| (3,2412) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 28       | 0.18          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 23       | 0.18          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 23       | 0.18          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 23       | 0.18          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 25       | 0.18          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 25       | 0.18          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 25       | 0.18          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 27       | 0.18          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 27       | 0.18          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 27       | 0.18          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 2        | 0.18          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 4        | 0.18          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 8        | 0.18          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 16       | 0.18          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 20       | 0.18          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 31       | 0.18          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 33       | 0.18          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 37       | 0.18          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 38       | 0.18          |
| (3,2351) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 40       | 0.18          |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 18       | 0.18          |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 19       | 0.18          |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 26       | 0.18          |
| (3,2289) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 28       | 0.18          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 9        | 0.18          |
| (3,2281) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 14       | 0.18          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1 | 9        | 0.18          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2 | 9        | 0.18          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1 | 10       | 0.18          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2 | 10       | 0.18          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1 | 11       | 0.18          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2 | 11       | 0.18          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1 | 23       | 0.18          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2 | 23       | 0.18          |
| (3,2173) | 1:43:A:TYR:HA  | 1:80:A:SER:H   | 11       | 0.18          |
| (3,2173) | 1:43:A:TYR:HA  | 1:80:A:SER:H   | 12       | 0.18          |
| (3,2173) | 1:43:A:TYR:HA  | 1:80:A:SER:H   | 22       | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 24       | 0.18          |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 38       | 0.18          |
| (3,2102) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HA   | 26       | 0.18          |
| (3,2102) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HA   | 26       | 0.18          |
| (3,2102) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HA   | 26       | 0.18          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 1        | 0.18          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 1        | 0.18          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 1        | 0.18          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 8        | 0.18          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 8        | 0.18          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 8        | 0.18          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 12       | 0.18          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 12       | 0.18          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 12       | 0.18          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 17       | 0.18          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 17       | 0.18          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 17       | 0.18          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 32       | 0.18          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 32       | 0.18          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 32       | 0.18          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1  | 35       | 0.18          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2  | 35       | 0.18          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1  | 35       | 0.18          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2  | 35       | 0.18          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1  | 35       | 0.18          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2  | 35       | 0.18          |
| (3,2075) | 1:97:A:LEU:HB2  | 1:19:A:ILE:HB   | 5        | 0.18          |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD11 | 4        | 0.18          |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD12 | 4        | 0.18          |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD13 | 4        | 0.18          |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD11 | 4        | 0.18          |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD12 | 4        | 0.18          |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD13 | 4        | 0.18          |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD11 | 4        | 0.18          |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD12 | 4        | 0.18          |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD13 | 4        | 0.18          |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD11 | 15       | 0.18          |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD12 | 15       | 0.18          |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD13 | 15       | 0.18          |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD11 | 15       | 0.18          |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD12 | 15       | 0.18          |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD13 | 15       | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD11 | 15       | 0.18          |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD12 | 15       | 0.18          |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD13 | 15       | 0.18          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 2        | 0.18          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 2        | 0.18          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 2        | 0.18          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 11       | 0.18          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 11       | 0.18          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 11       | 0.18          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 23       | 0.18          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 23       | 0.18          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 23       | 0.18          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 24       | 0.18          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 24       | 0.18          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 24       | 0.18          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 31       | 0.18          |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 27       | 0.18          |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 27       | 0.18          |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 27       | 0.18          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 3        | 0.18          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 4        | 0.18          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 27       | 0.18          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 34       | 0.18          |
| (3,1907) | 1:66:A:MET:HE1  | 1:43:A:TYR:H    | 33       | 0.18          |
| (3,1907) | 1:66:A:MET:HE2  | 1:43:A:TYR:H    | 33       | 0.18          |
| (3,1907) | 1:66:A:MET:HE3  | 1:43:A:TYR:H    | 33       | 0.18          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H    | 25       | 0.18          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H    | 25       | 0.18          |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H    | 25       | 0.18          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H    | 29       | 0.18          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H    | 29       | 0.18          |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H    | 29       | 0.18          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H    | 30       | 0.18          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H    | 30       | 0.18          |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H    | 30       | 0.18          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H    | 31       | 0.18          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H    | 31       | 0.18          |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H    | 31       | 0.18          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H    | 32       | 0.18          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H    | 32       | 0.18          |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H    | 32       | 0.18          |
| (3,1828) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HA   | 27       | 0.18          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,1828) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 29       | 0.18          |
| (3,1815) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 27       | 0.18          |
| (3,1815) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 29       | 0.18          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 3        | 0.18          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 5        | 0.18          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 6        | 0.18          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 7        | 0.18          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 8        | 0.18          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 14       | 0.18          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 15       | 0.18          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 16       | 0.18          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 17       | 0.18          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 19       | 0.18          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 24       | 0.18          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 26       | 0.18          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 35       | 0.18          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 37       | 0.18          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 40       | 0.18          |
| (3,1781) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 22       | 0.18          |
| (3,1781) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 23       | 0.18          |
| (3,1781) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 24       | 0.18          |
| (3,1781) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 28       | 0.18          |
| (3,1781) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 32       | 0.18          |
| (3,1781) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 34       | 0.18          |
| (3,1781) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 35       | 0.18          |
| (3,1747) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H   | 2        | 0.18          |
| (3,1747) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H   | 11       | 0.18          |
| (3,1747) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H   | 17       | 0.18          |
| (3,1747) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H   | 18       | 0.18          |
| (3,1747) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H   | 21       | 0.18          |
| (3,1747) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H   | 22       | 0.18          |
| (3,1747) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H   | 24       | 0.18          |
| (3,1747) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H   | 27       | 0.18          |
| (3,1747) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H   | 30       | 0.18          |
| (3,1747) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H   | 39       | 0.18          |
| (3,1731) | 1:48:A:GLU:HB2 | 1:48:A:GLU:H   | 1        | 0.18          |
| (3,1731) | 1:48:A:GLU:HB2 | 1:48:A:GLU:H   | 3        | 0.18          |
| (3,1731) | 1:48:A:GLU:HB2 | 1:48:A:GLU:H   | 8        | 0.18          |
| (3,1731) | 1:48:A:GLU:HB2 | 1:48:A:GLU:H   | 14       | 0.18          |
| (3,1731) | 1:48:A:GLU:HB2 | 1:48:A:GLU:H   | 22       | 0.18          |
| (3,1731) | 1:48:A:GLU:HB2 | 1:48:A:GLU:H   | 27       | 0.18          |
| (3,1731) | 1:48:A:GLU:HB2 | 1:48:A:GLU:H   | 32       | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1731) | 1:48:A:GLU:HB2  | 1:48:A:GLU:H    | 33       | 0.18          |
| (3,1731) | 1:48:A:GLU:HB2  | 1:48:A:GLU:H    | 38       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 11       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 11       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 11       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 11       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 11       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 11       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 11       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 11       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 11       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 22       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 22       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 22       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 22       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 22       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 22       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 22       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 22       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 22       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 25       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 25       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 25       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 25       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 25       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 25       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 25       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 25       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 25       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 34       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 34       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 34       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 34       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 34       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 34       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 34       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 34       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 34       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 39       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 39       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 39       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 39       | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 39       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 39       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 39       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 39       | 0.18          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 39       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 10       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 10       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 10       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 10       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 10       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 10       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 10       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 10       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 10       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 22       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 22       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 22       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 22       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 22       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 22       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 22       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 22       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 22       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 23       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 23       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 23       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 23       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 23       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 23       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 23       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 23       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 23       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 25       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 25       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 25       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 25       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 25       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 25       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 25       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 25       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 25       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 30       | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 30       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 30       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 30       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 30       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 30       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 30       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 30       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 30       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 34       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 34       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 34       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 34       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 34       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 34       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 34       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 34       | 0.18          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 34       | 0.18          |
| (3,1628) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2  | 38       | 0.18          |
| (3,1628) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2  | 38       | 0.18          |
| (3,1628) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2  | 38       | 0.18          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 1        | 0.18          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 1        | 0.18          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 1        | 0.18          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 3        | 0.18          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 3        | 0.18          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 3        | 0.18          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 4        | 0.18          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 4        | 0.18          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 4        | 0.18          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 5        | 0.18          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 5        | 0.18          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 5        | 0.18          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 6        | 0.18          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 6        | 0.18          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 6        | 0.18          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 7        | 0.18          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 7        | 0.18          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 7        | 0.18          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 9        | 0.18          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 9        | 0.18          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 9        | 0.18          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 10       | 0.18          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 10       | 0.18          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 10       | 0.18          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 26       | 0.18          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 26       | 0.18          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 26       | 0.18          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 28       | 0.18          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 28       | 0.18          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 28       | 0.18          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 31       | 0.18          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 31       | 0.18          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 31       | 0.18          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 35       | 0.18          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 35       | 0.18          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 35       | 0.18          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 36       | 0.18          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 36       | 0.18          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 36       | 0.18          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 38       | 0.18          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 38       | 0.18          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 38       | 0.18          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2 | 5        | 0.18          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 5        | 0.18          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 5        | 0.18          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2 | 8        | 0.18          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 8        | 0.18          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 8        | 0.18          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2 | 18       | 0.18          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 18       | 0.18          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 18       | 0.18          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2 | 40       | 0.18          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 40       | 0.18          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 40       | 0.18          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 1        | 0.18          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 1        | 0.18          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 1        | 0.18          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 1        | 0.18          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 1        | 0.18          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 1        | 0.18          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 16       | 0.18          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 16       | 0.18          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 16       | 0.18          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 16       | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 16       | 0.18          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 16       | 0.18          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 3        | 0.18          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 3        | 0.18          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 3        | 0.18          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 8        | 0.18          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 8        | 0.18          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 8        | 0.18          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 22       | 0.18          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 22       | 0.18          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 22       | 0.18          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 26       | 0.18          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 26       | 0.18          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 26       | 0.18          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 31       | 0.18          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 31       | 0.18          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 31       | 0.18          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 36       | 0.18          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 36       | 0.18          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 36       | 0.18          |
| (3,1582) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 3        | 0.18          |
| (3,1582) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 3        | 0.18          |
| (3,1582) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 3        | 0.18          |
| (3,1547) | 1:2:A:ILE:HG12  | 1:2:A:ILE:HA    | 23       | 0.18          |
| (3,1534) | 1:2:A:ILE:HG21  | 1:2:A:ILE:HA    | 10       | 0.18          |
| (3,1534) | 1:2:A:ILE:HG22  | 1:2:A:ILE:HA    | 10       | 0.18          |
| (3,1534) | 1:2:A:ILE:HG23  | 1:2:A:ILE:HA    | 10       | 0.18          |
| (3,1534) | 1:2:A:ILE:HG21  | 1:2:A:ILE:HA    | 14       | 0.18          |
| (3,1534) | 1:2:A:ILE:HG22  | 1:2:A:ILE:HA    | 14       | 0.18          |
| (3,1534) | 1:2:A:ILE:HG23  | 1:2:A:ILE:HA    | 14       | 0.18          |
| (3,1534) | 1:2:A:ILE:HG21  | 1:2:A:ILE:HA    | 17       | 0.18          |
| (3,1534) | 1:2:A:ILE:HG22  | 1:2:A:ILE:HA    | 17       | 0.18          |
| (3,1534) | 1:2:A:ILE:HG23  | 1:2:A:ILE:HA    | 17       | 0.18          |
| (3,1534) | 1:2:A:ILE:HG21  | 1:2:A:ILE:HA    | 23       | 0.18          |
| (3,1534) | 1:2:A:ILE:HG22  | 1:2:A:ILE:HA    | 23       | 0.18          |
| (3,1534) | 1:2:A:ILE:HG23  | 1:2:A:ILE:HA    | 23       | 0.18          |
| (3,1534) | 1:2:A:ILE:HG21  | 1:2:A:ILE:HA    | 37       | 0.18          |
| (3,1534) | 1:2:A:ILE:HG22  | 1:2:A:ILE:HA    | 37       | 0.18          |
| (3,1534) | 1:2:A:ILE:HG23  | 1:2:A:ILE:HA    | 37       | 0.18          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1  | 3        | 0.18          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2  | 3        | 0.18          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1  | 3        | 0.18          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2 | 3        | 0.18          |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1 | 3        | 0.18          |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2 | 3        | 0.18          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1 | 14       | 0.18          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2 | 14       | 0.18          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1 | 14       | 0.18          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2 | 14       | 0.18          |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1 | 14       | 0.18          |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2 | 14       | 0.18          |
| (3,1512) | 1:66:A:MET:HE1  | 1:42:A:TRP:HZ3 | 11       | 0.18          |
| (3,1512) | 1:66:A:MET:HE2  | 1:42:A:TRP:HZ3 | 11       | 0.18          |
| (3,1512) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3 | 11       | 0.18          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 2        | 0.18          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 2        | 0.18          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 2        | 0.18          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 5        | 0.18          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 5        | 0.18          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 5        | 0.18          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 38       | 0.18          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 38       | 0.18          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 38       | 0.18          |
| (3,1479) | 1:78:A:VAL:HG11 | 1:94:A:THR:HA  | 28       | 0.18          |
| (3,1479) | 1:78:A:VAL:HG12 | 1:94:A:THR:HA  | 28       | 0.18          |
| (3,1479) | 1:78:A:VAL:HG13 | 1:94:A:THR:HA  | 28       | 0.18          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 1        | 0.18          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 1        | 0.18          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 1        | 0.18          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 2        | 0.18          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 2        | 0.18          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 2        | 0.18          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 3        | 0.18          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 3        | 0.18          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 3        | 0.18          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 22       | 0.18          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 22       | 0.18          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 22       | 0.18          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 27       | 0.18          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 27       | 0.18          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 27       | 0.18          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 38       | 0.18          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 38       | 0.18          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 38       | 0.18          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 2        | 0.18          |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 2        | 0.18          |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 2        | 0.18          |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 14       | 0.18          |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 14       | 0.18          |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 14       | 0.18          |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 20       | 0.18          |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 20       | 0.18          |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 20       | 0.18          |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 35       | 0.18          |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 35       | 0.18          |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 35       | 0.18          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 4        | 0.18          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 4        | 0.18          |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 4        | 0.18          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 20       | 0.18          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 20       | 0.18          |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 20       | 0.18          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 24       | 0.18          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 24       | 0.18          |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 24       | 0.18          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 28       | 0.18          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 28       | 0.18          |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 28       | 0.18          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 33       | 0.18          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 33       | 0.18          |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 33       | 0.18          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 34       | 0.18          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 34       | 0.18          |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 34       | 0.18          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H   | 8        | 0.18          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H   | 8        | 0.18          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H   | 8        | 0.18          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H   | 12       | 0.18          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H   | 12       | 0.18          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H   | 12       | 0.18          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H   | 13       | 0.18          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H   | 13       | 0.18          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H   | 13       | 0.18          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H   | 24       | 0.18          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H   | 24       | 0.18          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H   | 24       | 0.18          |

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| Key      | Atom-1          | Atom-2       | Model ID | Violation (Å) |
|----------|-----------------|--------------|----------|---------------|
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 31       | 0.18          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 31       | 0.18          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 31       | 0.18          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 38       | 0.18          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 38       | 0.18          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 38       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 7        | 0.18          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 7        | 0.18          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 7        | 0.18          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 11       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 11       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 11       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 14       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 14       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 14       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 16       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 16       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 16       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 18       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 18       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 18       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 19       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 19       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 19       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 21       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 21       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 21       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 22       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 22       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 22       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 24       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 24       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 24       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 25       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 25       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 25       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 26       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 26       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 26       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 27       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 27       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 27       | 0.18          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H  | 30       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H  | 30       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H  | 30       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H  | 31       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H  | 31       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H  | 31       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H  | 33       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H  | 33       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H  | 33       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H  | 35       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H  | 35       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H  | 35       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H  | 36       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H  | 36       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H  | 36       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H  | 37       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H  | 37       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H  | 37       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H  | 38       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H  | 38       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H  | 38       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H  | 40       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H  | 40       | 0.18          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H  | 40       | 0.18          |
| (3,1405) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H  | 6        | 0.18          |
| (3,1405) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H  | 6        | 0.18          |
| (3,1405) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H  | 6        | 0.18          |
| (3,1405) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H  | 37       | 0.18          |
| (3,1405) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H  | 37       | 0.18          |
| (3,1405) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H  | 37       | 0.18          |
| (3,1400) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA | 2        | 0.18          |
| (3,1400) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA | 2        | 0.18          |
| (3,1400) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA | 2        | 0.18          |
| (3,1400) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA | 15       | 0.18          |
| (3,1400) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA | 15       | 0.18          |
| (3,1400) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA | 15       | 0.18          |
| (3,1400) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA | 22       | 0.18          |
| (3,1400) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA | 22       | 0.18          |
| (3,1400) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA | 22       | 0.18          |
| (3,1391) | 1:91:A:ALA:HB1  | 1:12:A:PHE:HZ | 20       | 0.18          |
| (3,1391) | 1:91:A:ALA:HB2  | 1:12:A:PHE:HZ | 20       | 0.18          |
| (3,1391) | 1:91:A:ALA:HB3  | 1:12:A:PHE:HZ | 20       | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1391) | 1:91:A:ALA:HB1  | 1:12:A:PHE:HZ   | 38       | 0.18          |
| (3,1391) | 1:91:A:ALA:HB2  | 1:12:A:PHE:HZ   | 38       | 0.18          |
| (3,1391) | 1:91:A:ALA:HB3  | 1:12:A:PHE:HZ   | 38       | 0.18          |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 8        | 0.18          |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 23       | 0.18          |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 25       | 0.18          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 9        | 0.18          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 9        | 0.18          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 9        | 0.18          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 13       | 0.18          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 13       | 0.18          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 13       | 0.18          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 13       | 0.18          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 13       | 0.18          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 13       | 0.18          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 13       | 0.18          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 13       | 0.18          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 13       | 0.18          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 20       | 0.18          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 20       | 0.18          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 20       | 0.18          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 20       | 0.18          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 20       | 0.18          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 20       | 0.18          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 20       | 0.18          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 20       | 0.18          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 20       | 0.18          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 4        | 0.18          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 4        | 0.18          |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 4        | 0.18          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 5        | 0.18          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 5        | 0.18          |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 5        | 0.18          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 11       | 0.18          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 11       | 0.18          |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 11       | 0.18          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 13       | 0.18          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 13       | 0.18          |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 13       | 0.18          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 31       | 0.18          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 31       | 0.18          |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 31       | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 4        | 0.18          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 4        | 0.18          |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 4        | 0.18          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 5        | 0.18          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 5        | 0.18          |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 5        | 0.18          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 11       | 0.18          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 11       | 0.18          |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 11       | 0.18          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 13       | 0.18          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 13       | 0.18          |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 13       | 0.18          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 31       | 0.18          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 31       | 0.18          |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 31       | 0.18          |
| (3,1261) | 1:67:A:THR:HG21 | 1:26:A:SER:HB2  | 6        | 0.18          |
| (3,1261) | 1:67:A:THR:HG22 | 1:26:A:SER:HB2  | 6        | 0.18          |
| (3,1261) | 1:67:A:THR:HG23 | 1:26:A:SER:HB2  | 6        | 0.18          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 3        | 0.18          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 3        | 0.18          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 3        | 0.18          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 13       | 0.18          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 13       | 0.18          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 13       | 0.18          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 18       | 0.18          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 18       | 0.18          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 18       | 0.18          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 5        | 0.18          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 5        | 0.18          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 5        | 0.18          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 31       | 0.18          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 31       | 0.18          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 31       | 0.18          |
| (3,1240) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3  | 28       | 0.18          |
| (3,1240) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3  | 28       | 0.18          |
| (3,1240) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3  | 28       | 0.18          |
| (3,1217) | 1:66:A:MET:H    | 1:28:A:THR:HA   | 10       | 0.18          |
| (3,1217) | 1:66:A:MET:H    | 1:28:A:THR:HA   | 26       | 0.18          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 1        | 0.18          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 1        | 0.18          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 1        | 0.18          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 2        | 0.18          |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (3,1194) | 1:22:A:SER:H  | 1:21:A:VAL:HG22 | 2        | 0.18          |
| (3,1194) | 1:22:A:SER:H  | 1:21:A:VAL:HG23 | 2        | 0.18          |
| (3,1194) | 1:22:A:SER:H  | 1:21:A:VAL:HG21 | 12       | 0.18          |
| (3,1194) | 1:22:A:SER:H  | 1:21:A:VAL:HG22 | 12       | 0.18          |
| (3,1194) | 1:22:A:SER:H  | 1:21:A:VAL:HG23 | 12       | 0.18          |
| (3,1194) | 1:22:A:SER:H  | 1:21:A:VAL:HG21 | 13       | 0.18          |
| (3,1194) | 1:22:A:SER:H  | 1:21:A:VAL:HG22 | 13       | 0.18          |
| (3,1194) | 1:22:A:SER:H  | 1:21:A:VAL:HG23 | 13       | 0.18          |
| (3,1194) | 1:22:A:SER:H  | 1:21:A:VAL:HG21 | 26       | 0.18          |
| (3,1194) | 1:22:A:SER:H  | 1:21:A:VAL:HG22 | 26       | 0.18          |
| (3,1194) | 1:22:A:SER:H  | 1:21:A:VAL:HG23 | 26       | 0.18          |
| (3,1194) | 1:22:A:SER:H  | 1:21:A:VAL:HG21 | 28       | 0.18          |
| (3,1194) | 1:22:A:SER:H  | 1:21:A:VAL:HG22 | 28       | 0.18          |
| (3,1194) | 1:22:A:SER:H  | 1:21:A:VAL:HG23 | 28       | 0.18          |
| (3,1189) | 1:21:A:VAL:H  | 1:100:A:GLU:HB3 | 2        | 0.18          |
| (3,1189) | 1:21:A:VAL:H  | 1:100:A:GLU:HB3 | 6        | 0.18          |
| (3,1189) | 1:21:A:VAL:H  | 1:100:A:GLU:HB3 | 13       | 0.18          |
| (3,1189) | 1:21:A:VAL:H  | 1:100:A:GLU:HB3 | 33       | 0.18          |
| (3,1189) | 1:21:A:VAL:H  | 1:100:A:GLU:HB3 | 34       | 0.18          |
| (3,1173) | 1:14:A:LYS:H  | 1:14:A:LYS:HD2  | 23       | 0.18          |
| (3,1173) | 1:14:A:LYS:H  | 1:14:A:LYS:HD2  | 27       | 0.18          |
| (3,1173) | 1:14:A:LYS:H  | 1:14:A:LYS:HD2  | 32       | 0.18          |
| (3,1173) | 1:14:A:LYS:H  | 1:14:A:LYS:HD2  | 37       | 0.18          |
| (3,1167) | 1:75:A:ASP:H  | 1:74:A:ASP:HB2  | 29       | 0.18          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 12       | 0.18          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 12       | 0.18          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 24       | 0.18          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 24       | 0.18          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 29       | 0.18          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 29       | 0.18          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 35       | 0.18          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 35       | 0.18          |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 5        | 0.18          |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 7        | 0.18          |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 11       | 0.18          |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 13       | 0.18          |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 26       | 0.18          |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 27       | 0.18          |
| (3,1096) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 1        | 0.18          |
| (3,1096) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 2        | 0.18          |
| (3,1096) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 4        | 0.18          |
| (3,1096) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 9        | 0.18          |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (3,1096) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 16       | 0.18          |
| (3,1096) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 20       | 0.18          |
| (3,1019) | 1:48:A:GLU:H  | 1:48:A:GLU:HG3  | 37       | 0.18          |
| (3,963)  | 1:102:A:ARG:H | 1:101:A:LEU:HB2 | 23       | 0.18          |
| (3,942)  | 1:34:A:SER:H  | 1:12:A:PHE:HA   | 28       | 0.18          |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 3        | 0.18          |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 7        | 0.18          |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 10       | 0.18          |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 12       | 0.18          |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 16       | 0.18          |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 22       | 0.18          |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 23       | 0.18          |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 26       | 0.18          |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 28       | 0.18          |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 31       | 0.18          |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 32       | 0.18          |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 36       | 0.18          |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 40       | 0.18          |
| (3,919)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB3  | 24       | 0.18          |
| (3,919)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB3  | 38       | 0.18          |
| (3,889)  | 1:80:A:SER:H  | 1:43:A:TYR:HB3  | 18       | 0.18          |
| (3,889)  | 1:80:A:SER:H  | 1:43:A:TYR:HB3  | 34       | 0.18          |
| (3,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3   | 1        | 0.18          |
| (3,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3   | 3        | 0.18          |
| (3,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3   | 4        | 0.18          |
| (3,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3   | 14       | 0.18          |
| (3,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3   | 17       | 0.18          |
| (3,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3   | 19       | 0.18          |
| (3,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3   | 33       | 0.18          |
| (3,870)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD2   | 22       | 0.18          |
| (3,870)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD2   | 27       | 0.18          |
| (3,870)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD2   | 35       | 0.18          |
| (3,870)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD2   | 38       | 0.18          |
| (3,869)  | 1:8:A:GLU:H   | 1:7:A:ALA:HA    | 1        | 0.18          |
| (3,869)  | 1:8:A:GLU:H   | 1:7:A:ALA:HA    | 3        | 0.18          |
| (3,869)  | 1:8:A:GLU:H   | 1:7:A:ALA:HA    | 15       | 0.18          |
| (3,869)  | 1:8:A:GLU:H   | 1:7:A:ALA:HA    | 18       | 0.18          |
| (3,869)  | 1:8:A:GLU:H   | 1:7:A:ALA:HA    | 24       | 0.18          |
| (3,869)  | 1:8:A:GLU:H   | 1:7:A:ALA:HA    | 38       | 0.18          |
| (3,849)  | 1:83:A:ALA:H  | 1:91:A:ALA:HB1  | 37       | 0.18          |
| (3,849)  | 1:83:A:ALA:H  | 1:91:A:ALA:HB2  | 37       | 0.18          |
| (3,849)  | 1:83:A:ALA:H  | 1:91:A:ALA:HB3  | 37       | 0.18          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (3,847) | 1:83:A:ALA:H  | 1:83:A:ALA:HA   | 7        | 0.18          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG21 | 4        | 0.18          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG22 | 4        | 0.18          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG23 | 4        | 0.18          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG21 | 13       | 0.18          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG22 | 13       | 0.18          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG23 | 13       | 0.18          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG21 | 35       | 0.18          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG22 | 35       | 0.18          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG23 | 35       | 0.18          |
| (3,810) | 1:25:A:GLN:H  | 1:71:A:VAL:HB   | 8        | 0.18          |
| (3,801) | 1:54:A:LYS:H  | 1:54:A:LYS:HD2  | 1        | 0.18          |
| (3,801) | 1:54:A:LYS:H  | 1:54:A:LYS:HD2  | 6        | 0.18          |
| (3,801) | 1:54:A:LYS:H  | 1:54:A:LYS:HD2  | 8        | 0.18          |
| (3,801) | 1:54:A:LYS:H  | 1:54:A:LYS:HD2  | 14       | 0.18          |
| (3,801) | 1:54:A:LYS:H  | 1:54:A:LYS:HD2  | 39       | 0.18          |
| (3,786) | 1:6:A:THR:H   | 1:6:A:THR:HG21  | 6        | 0.18          |
| (3,786) | 1:6:A:THR:H   | 1:6:A:THR:HG22  | 6        | 0.18          |
| (3,786) | 1:6:A:THR:H   | 1:6:A:THR:HG23  | 6        | 0.18          |
| (3,783) | 1:74:A:ASP:H  | 1:74:A:ASP:HB3  | 36       | 0.18          |
| (3,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 1        | 0.18          |
| (3,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 6        | 0.18          |
| (3,739) | 1:15:A:ARG:H  | 1:14:A:LYS:HB2  | 23       | 0.18          |
| (3,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 3        | 0.18          |
| (3,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 20       | 0.18          |
| (3,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 40       | 0.18          |
| (3,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 20       | 0.18          |
| (3,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 9        | 0.18          |
| (3,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 12       | 0.18          |
| (3,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 27       | 0.18          |
| (3,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 28       | 0.18          |
| (3,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 38       | 0.18          |
| (3,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3  | 22       | 0.18          |
| (3,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3  | 33       | 0.18          |
| (3,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3  | 34       | 0.18          |
| (3,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3  | 35       | 0.18          |
| (3,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3  | 37       | 0.18          |
| (3,684) | 1:23:A:GLU:H  | 1:23:A:GLU:HB3  | 24       | 0.18          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 2        | 0.18          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 22       | 0.18          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 9        | 0.18          |
| (3,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 3        | 0.18          |

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| Key     | Atom-1       | Atom-2         | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (3,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 9        | 0.18          |
| (3,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 18       | 0.18          |
| (3,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 26       | 0.18          |
| (3,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 30       | 0.18          |
| (3,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 38       | 0.18          |
| (3,589) | 1:93:A:SER:H | 1:92:A:ARG:HG2 | 2        | 0.18          |
| (3,589) | 1:93:A:SER:H | 1:92:A:ARG:HG2 | 5        | 0.18          |
| (3,589) | 1:93:A:SER:H | 1:92:A:ARG:HG2 | 9        | 0.18          |
| (3,589) | 1:93:A:SER:H | 1:92:A:ARG:HG2 | 11       | 0.18          |
| (3,589) | 1:93:A:SER:H | 1:92:A:ARG:HG2 | 24       | 0.18          |
| (3,589) | 1:93:A:SER:H | 1:92:A:ARG:HG2 | 25       | 0.18          |
| (3,589) | 1:93:A:SER:H | 1:92:A:ARG:HG2 | 30       | 0.18          |
| (3,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 1        | 0.18          |
| (3,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 7        | 0.18          |
| (3,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 12       | 0.18          |
| (3,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 17       | 0.18          |
| (3,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 29       | 0.18          |
| (3,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 30       | 0.18          |
| (3,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 37       | 0.18          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1 | 9        | 0.18          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2 | 9        | 0.18          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1 | 11       | 0.18          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2 | 11       | 0.18          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1 | 14       | 0.18          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2 | 14       | 0.18          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1 | 15       | 0.18          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2 | 15       | 0.18          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1 | 39       | 0.18          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2 | 39       | 0.18          |
| (3,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA  | 3        | 0.18          |
| (3,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA  | 26       | 0.18          |
| (3,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA  | 34       | 0.18          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 1        | 0.18          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 2        | 0.18          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 5        | 0.18          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 8        | 0.18          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 20       | 0.18          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 21       | 0.18          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 24       | 0.18          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 27       | 0.18          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 28       | 0.18          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 31       | 0.18          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 9        | 0.18          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 15       | 0.18          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 21       | 0.18          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 8        | 0.18          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 11       | 0.18          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 13       | 0.18          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 21       | 0.18          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 23       | 0.18          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 25       | 0.18          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 26       | 0.18          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 30       | 0.18          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 35       | 0.18          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 36       | 0.18          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 3        | 0.18          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 8        | 0.18          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 14       | 0.18          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 20       | 0.18          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 35       | 0.18          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 37       | 0.18          |
| (3,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 3        | 0.18          |
| (3,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 22       | 0.18          |
| (3,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 23       | 0.18          |
| (3,410) | 1:96:A:GLU:H | 1:18:A:ASN:HD21 | 29       | 0.18          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 8        | 0.18          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 17       | 0.18          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 24       | 0.18          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 29       | 0.18          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 30       | 0.18          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 32       | 0.18          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 33       | 0.18          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 40       | 0.18          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 27       | 0.18          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 27       | 0.18          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 27       | 0.18          |
| (3,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 18       | 0.18          |
| (3,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 29       | 0.18          |
| (3,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 31       | 0.18          |
| (3,274) | 1:66:A:MET:H | 1:66:A:MET:HG3  | 7        | 0.18          |
| (3,274) | 1:66:A:MET:H | 1:66:A:MET:HG3  | 15       | 0.18          |
| (3,274) | 1:66:A:MET:H | 1:66:A:MET:HG3  | 24       | 0.18          |
| (3,274) | 1:66:A:MET:H | 1:66:A:MET:HG3  | 29       | 0.18          |
| (3,274) | 1:66:A:MET:H | 1:66:A:MET:HG3  | 33       | 0.18          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (3,274) | 1:66:A:MET:H  | 1:66:A:MET:HG3  | 39       | 0.18          |
| (3,274) | 1:66:A:MET:H  | 1:66:A:MET:HG3  | 40       | 0.18          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 4        | 0.18          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 4        | 0.18          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 4        | 0.18          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 5        | 0.18          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 5        | 0.18          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 5        | 0.18          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 11       | 0.18          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 11       | 0.18          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 11       | 0.18          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 13       | 0.18          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 13       | 0.18          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 13       | 0.18          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 31       | 0.18          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 31       | 0.18          |
| (3,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 31       | 0.18          |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 2        | 0.18          |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 3        | 0.18          |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 5        | 0.18          |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 6        | 0.18          |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 8        | 0.18          |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 10       | 0.18          |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 12       | 0.18          |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 14       | 0.18          |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 16       | 0.18          |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 19       | 0.18          |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 21       | 0.18          |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 22       | 0.18          |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 24       | 0.18          |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 27       | 0.18          |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 28       | 0.18          |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 31       | 0.18          |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 33       | 0.18          |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 35       | 0.18          |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 36       | 0.18          |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 38       | 0.18          |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 39       | 0.18          |
| (3,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 1        | 0.18          |
| (3,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 37       | 0.18          |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 5        | 0.18          |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 7        | 0.18          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 11       | 0.18          |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 13       | 0.18          |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 26       | 0.18          |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 27       | 0.18          |
| (3,135) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 6        | 0.18          |
| (3,135) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 9        | 0.18          |
| (3,135) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 21       | 0.18          |
| (3,135) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 39       | 0.18          |
| (3,131) | 1:39:A:ILE:H  | 1:39:A:ILE:HA   | 2        | 0.18          |
| (3,131) | 1:39:A:ILE:H  | 1:39:A:ILE:HA   | 11       | 0.18          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 1        | 0.18          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 2        | 0.18          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 10       | 0.18          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 13       | 0.18          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 17       | 0.18          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 18       | 0.18          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 21       | 0.18          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 22       | 0.18          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 23       | 0.18          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 25       | 0.18          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 26       | 0.18          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 27       | 0.18          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 28       | 0.18          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 30       | 0.18          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 33       | 0.18          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 36       | 0.18          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 40       | 0.18          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 2        | 0.18          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 11       | 0.18          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 17       | 0.18          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 18       | 0.18          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 21       | 0.18          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 22       | 0.18          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 24       | 0.18          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 27       | 0.18          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 30       | 0.18          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 39       | 0.18          |
| (3,59)  | 1:42:A:TRP:H  | 1:41:A:THR:HB   | 1        | 0.18          |
| (3,59)  | 1:42:A:TRP:H  | 1:41:A:THR:HB   | 3        | 0.18          |
| (3,59)  | 1:42:A:TRP:H  | 1:41:A:THR:HB   | 8        | 0.18          |
| (3,59)  | 1:42:A:TRP:H  | 1:41:A:THR:HB   | 15       | 0.18          |
| (3,59)  | 1:42:A:TRP:H  | 1:41:A:THR:HB   | 27       | 0.18          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,51)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2  | 2        | 0.18          |
| (3,51)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2  | 5        | 0.18          |
| (3,51)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2  | 9        | 0.18          |
| (3,51)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2  | 11       | 0.18          |
| (3,51)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2  | 13       | 0.18          |
| (3,51)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2  | 21       | 0.18          |
| (3,51)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2  | 23       | 0.18          |
| (3,51)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2  | 29       | 0.18          |
| (3,51)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2  | 32       | 0.18          |
| (3,51)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2  | 33       | 0.18          |
| (3,51)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2  | 37       | 0.18          |
| (3,51)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2  | 38       | 0.18          |
| (3,51)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2  | 39       | 0.18          |
| (3,22)   | 1:89:A:GLY:H   | 1:85:A:LEU:H    | 23       | 0.18          |
| (3,22)   | 1:89:A:GLY:H   | 1:85:A:LEU:H    | 29       | 0.18          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 7        | 0.18          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 7        | 0.18          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 14       | 0.18          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 14       | 0.18          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 34       | 0.18          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 34       | 0.18          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 12       | 0.18          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 12       | 0.18          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 12       | 0.18          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 12       | 0.18          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 12       | 0.18          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 12       | 0.18          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 16       | 0.18          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 16       | 0.18          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 16       | 0.18          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 16       | 0.18          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 16       | 0.18          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 16       | 0.18          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 24       | 0.18          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 24       | 0.18          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 24       | 0.18          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 24       | 0.18          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 24       | 0.18          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 24       | 0.18          |
| (1,3199) | 1:43:A:TYR:HD1 | 1:80:A:SER:HB2  | 34       | 0.18          |
| (1,3199) | 1:43:A:TYR:HD2 | 1:80:A:SER:HB2  | 34       | 0.18          |
| (1,3199) | 1:43:A:TYR:HD1 | 1:80:A:SER:HB2  | 37       | 0.18          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,3199) | 1:43:A:TYR:HD2 | 1:80:A:SER:HB2 | 37       | 0.18          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1 | 6        | 0.18          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2 | 6        | 0.18          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1 | 6        | 0.18          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2 | 6        | 0.18          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1 | 12       | 0.18          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2 | 12       | 0.18          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1 | 12       | 0.18          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2 | 12       | 0.18          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB  | 3        | 0.18          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB  | 12       | 0.18          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB  | 23       | 0.18          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB  | 27       | 0.18          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB  | 28       | 0.18          |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 9        | 0.18          |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 9        | 0.18          |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 15       | 0.18          |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 15       | 0.18          |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 29       | 0.18          |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 29       | 0.18          |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 39       | 0.18          |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 39       | 0.18          |
| (1,3132) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB2 | 20       | 0.18          |
| (1,3132) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB2 | 20       | 0.18          |
| (1,3131) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3 | 22       | 0.18          |
| (1,3131) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3 | 22       | 0.18          |
| (1,3131) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3 | 25       | 0.18          |
| (1,3131) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3 | 25       | 0.18          |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2 | 31       | 0.18          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2 | 31       | 0.18          |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2 | 32       | 0.18          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2 | 32       | 0.18          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 5        | 0.18          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 5        | 0.18          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 10       | 0.18          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 10       | 0.18          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 21       | 0.18          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 21       | 0.18          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 24       | 0.18          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 24       | 0.18          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 31       | 0.18          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 31       | 0.18          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 34       | 0.18          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 34       | 0.18          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 5        | 0.18          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 5        | 0.18          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 10       | 0.18          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 10       | 0.18          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 21       | 0.18          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 21       | 0.18          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 24       | 0.18          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 24       | 0.18          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 31       | 0.18          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 31       | 0.18          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 34       | 0.18          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 34       | 0.18          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 1        | 0.18          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 1        | 0.18          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 1        | 0.18          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 1        | 0.18          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 1        | 0.18          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 1        | 0.18          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 36       | 0.18          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 36       | 0.18          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 36       | 0.18          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 36       | 0.18          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 36       | 0.18          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 36       | 0.18          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 6        | 0.18          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 6        | 0.18          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 6        | 0.18          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 6        | 0.18          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 6        | 0.18          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 6        | 0.18          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 17       | 0.18          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 17       | 0.18          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 17       | 0.18          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 17       | 0.18          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 17       | 0.18          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 17       | 0.18          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 28       | 0.18          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 28       | 0.18          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 28       | 0.18          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 28       | 0.18          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 28       | 0.18          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 28       | 0.18          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 7        | 0.18          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 8        | 0.18          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 12       | 0.18          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 16       | 0.18          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 18       | 0.18          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 20       | 0.18          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 3        | 0.18          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 3        | 0.18          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 3        | 0.18          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 17       | 0.18          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 17       | 0.18          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 17       | 0.18          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 5        | 0.18          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 5        | 0.18          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 8        | 0.18          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 8        | 0.18          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB2  | 22       | 0.18          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB3  | 22       | 0.18          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB2  | 33       | 0.18          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB3  | 33       | 0.18          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB2  | 40       | 0.18          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB3  | 40       | 0.18          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 5        | 0.18          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 7        | 0.18          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 8        | 0.18          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 11       | 0.18          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 19       | 0.18          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 26       | 0.18          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 32       | 0.18          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 36       | 0.18          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 40       | 0.18          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 7        | 0.18          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 7        | 0.18          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 7        | 0.18          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 10       | 0.18          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 10       | 0.18          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 10       | 0.18          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 16       | 0.18          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 16       | 0.18          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 16       | 0.18          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 21       | 0.18          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 21       | 0.18          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 21       | 0.18          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 25       | 0.18          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 25       | 0.18          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 25       | 0.18          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 28       | 0.18          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 28       | 0.18          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 28       | 0.18          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 31       | 0.18          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 31       | 0.18          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 31       | 0.18          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 32       | 0.18          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 32       | 0.18          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 32       | 0.18          |
| (1,2996) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 13       | 0.18          |
| (1,2996) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 19       | 0.18          |
| (1,2931) | 1:26:A:SER:HA  | 1:70:A:ASN:H    | 1        | 0.18          |
| (1,2931) | 1:26:A:SER:HA  | 1:70:A:ASN:H    | 18       | 0.18          |
| (1,2931) | 1:26:A:SER:HA  | 1:70:A:ASN:H    | 39       | 0.18          |
| (1,2918) | 1:22:A:SER:HB2 | 1:25:A:GLN:H    | 15       | 0.18          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 3        | 0.18          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 5        | 0.18          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 6        | 0.18          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 7        | 0.18          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 8        | 0.18          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 14       | 0.18          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 15       | 0.18          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 16       | 0.18          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 17       | 0.18          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 19       | 0.18          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 24       | 0.18          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 26       | 0.18          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 35       | 0.18          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 37       | 0.18          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 40       | 0.18          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3  | 3        | 0.18          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3  | 5        | 0.18          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3  | 6        | 0.18          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3  | 7        | 0.18          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3  | 8        | 0.18          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3  | 14       | 0.18          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2904) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HE3 | 15       | 0.18          |
| (1,2904) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HE3 | 16       | 0.18          |
| (1,2904) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HE3 | 17       | 0.18          |
| (1,2904) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HE3 | 19       | 0.18          |
| (1,2904) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HE3 | 24       | 0.18          |
| (1,2904) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HE3 | 26       | 0.18          |
| (1,2904) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HE3 | 35       | 0.18          |
| (1,2904) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HE3 | 37       | 0.18          |
| (1,2904) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HE3 | 40       | 0.18          |
| (1,2802) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HB2 | 17       | 0.18          |
| (1,2802) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HB2 | 26       | 0.18          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H  | 2        | 0.18          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H  | 22       | 0.18          |
| (1,2754) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H   | 26       | 0.18          |
| (1,2745) | 1:86:A:GLU:HG2  | 1:86:A:GLU:H   | 27       | 0.18          |
| (1,2745) | 1:86:A:GLU:HG3  | 1:86:A:GLU:H   | 27       | 0.18          |
| (1,2686) | 1:8:A:GLU:HB3   | 1:8:A:GLU:HG2  | 2        | 0.18          |
| (1,2685) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 1        | 0.18          |
| (1,2685) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 2        | 0.18          |
| (1,2685) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 4        | 0.18          |
| (1,2685) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 5        | 0.18          |
| (1,2685) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 8        | 0.18          |
| (1,2685) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 9        | 0.18          |
| (1,2685) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 14       | 0.18          |
| (1,2685) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 17       | 0.18          |
| (1,2685) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 18       | 0.18          |
| (1,2685) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 19       | 0.18          |
| (1,2685) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 20       | 0.18          |
| (1,2685) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 23       | 0.18          |
| (1,2685) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 27       | 0.18          |
| (1,2685) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 35       | 0.18          |
| (1,2685) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 37       | 0.18          |
| (1,2685) | 1:8:A:GLU:HB2   | 1:8:A:GLU:HG2  | 38       | 0.18          |
| (1,2675) | 1:25:A:GLN:HG3  | 1:26:A:SER:H   | 26       | 0.18          |
| (1,2645) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3  | 33       | 0.18          |
| (1,2631) | 1:11:A:GLN:HB3  | 1:11:A:GLN:HG3 | 18       | 0.18          |
| (1,2615) | 1:74:A:ASP:HB3  | 1:74:A:ASP:H   | 36       | 0.18          |
| (1,2597) | 1:36:A:ASP:HB3  | 1:37:A:ASP:H   | 24       | 0.18          |
| (1,2597) | 1:36:A:ASP:HB3  | 1:37:A:ASP:H   | 38       | 0.18          |
| (1,2550) | 1:92:A:ARG:HA   | 1:83:A:ALA:H   | 17       | 0.18          |
| (1,2550) | 1:92:A:ARG:HA   | 1:83:A:ALA:H   | 21       | 0.18          |
| (1,2537) | 1:73:A:PRO:HG3  | 1:73:A:PRO:HA  | 31       | 0.18          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,2511) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 1        | 0.18          |
| (1,2511) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 2        | 0.18          |
| (1,2511) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 3        | 0.18          |
| (1,2511) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 4        | 0.18          |
| (1,2511) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 5        | 0.18          |
| (1,2511) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 6        | 0.18          |
| (1,2511) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 8        | 0.18          |
| (1,2511) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 15       | 0.18          |
| (1,2511) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 18       | 0.18          |
| (1,2511) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 20       | 0.18          |
| (1,2460) | 1:4:A:PRO:HD3  | 1:3:A:ASP:HA   | 6        | 0.18          |
| (1,2460) | 1:4:A:PRO:HD3  | 1:3:A:ASP:HA   | 22       | 0.18          |
| (1,2431) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 1        | 0.18          |
| (1,2431) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 13       | 0.18          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 8        | 0.18          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 28       | 0.18          |
| (1,2402) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 23       | 0.18          |
| (1,2402) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 23       | 0.18          |
| (1,2402) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 23       | 0.18          |
| (1,2402) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 25       | 0.18          |
| (1,2402) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 25       | 0.18          |
| (1,2402) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 25       | 0.18          |
| (1,2402) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 27       | 0.18          |
| (1,2402) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 27       | 0.18          |
| (1,2402) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 27       | 0.18          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 2        | 0.18          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 4        | 0.18          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 8        | 0.18          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 16       | 0.18          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 20       | 0.18          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 31       | 0.18          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 33       | 0.18          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 37       | 0.18          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 38       | 0.18          |
| (1,2348) | 1:21:A:VAL:HB  | 1:21:A:VAL:HA  | 40       | 0.18          |
| (1,2286) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 18       | 0.18          |
| (1,2286) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 19       | 0.18          |
| (1,2286) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 26       | 0.18          |
| (1,2286) | 1:96:A:GLU:HG2 | 1:97:A:LEU:H   | 28       | 0.18          |
| (1,2278) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 9        | 0.18          |
| (1,2278) | 1:96:A:GLU:HG3 | 1:96:A:GLU:HB3 | 14       | 0.18          |
| (1,2250) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1 | 9        | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 9        | 0.18          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 10       | 0.18          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 10       | 0.18          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 11       | 0.18          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 11       | 0.18          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 23       | 0.18          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 23       | 0.18          |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 11       | 0.18          |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 12       | 0.18          |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 22       | 0.18          |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 24       | 0.18          |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 38       | 0.18          |
| (1,2099) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HA   | 26       | 0.18          |
| (1,2099) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HA   | 26       | 0.18          |
| (1,2099) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HA   | 26       | 0.18          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 1        | 0.18          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 1        | 0.18          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 1        | 0.18          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 8        | 0.18          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 8        | 0.18          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 8        | 0.18          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 12       | 0.18          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 12       | 0.18          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 12       | 0.18          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 17       | 0.18          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 17       | 0.18          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 17       | 0.18          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 32       | 0.18          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 32       | 0.18          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 32       | 0.18          |
| (1,2087) | 1:85:A:LEU:HD11 | 1:39:A:ILE:H    | 11       | 0.18          |
| (1,2087) | 1:85:A:LEU:HD12 | 1:39:A:ILE:H    | 11       | 0.18          |
| (1,2087) | 1:85:A:LEU:HD13 | 1:39:A:ILE:H    | 11       | 0.18          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1  | 35       | 0.18          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2  | 35       | 0.18          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1  | 35       | 0.18          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2  | 35       | 0.18          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1  | 35       | 0.18          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2  | 35       | 0.18          |
| (1,2070) | 1:97:A:LEU:HB2  | 1:19:A:ILE:HB   | 5        | 0.18          |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD11 | 4        | 0.18          |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD12 | 4        | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD13 | 4        | 0.18          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD11 | 4        | 0.18          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD12 | 4        | 0.18          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD13 | 4        | 0.18          |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD11 | 4        | 0.18          |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD12 | 4        | 0.18          |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD13 | 4        | 0.18          |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD11 | 15       | 0.18          |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD12 | 15       | 0.18          |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD13 | 15       | 0.18          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD11 | 15       | 0.18          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD12 | 15       | 0.18          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD13 | 15       | 0.18          |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD11 | 15       | 0.18          |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD12 | 15       | 0.18          |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD13 | 15       | 0.18          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3  | 4        | 0.18          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3  | 4        | 0.18          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3  | 4        | 0.18          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 2        | 0.18          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 2        | 0.18          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 2        | 0.18          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 11       | 0.18          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 11       | 0.18          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 11       | 0.18          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 23       | 0.18          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 23       | 0.18          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 23       | 0.18          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 24       | 0.18          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 24       | 0.18          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 24       | 0.18          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 31       | 0.18          |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 27       | 0.18          |
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 27       | 0.18          |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 27       | 0.18          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 3        | 0.18          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 4        | 0.18          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 27       | 0.18          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 34       | 0.18          |
| (1,1904) | 1:66:A:MET:HE1  | 1:43:A:TYR:H    | 33       | 0.18          |
| (1,1904) | 1:66:A:MET:HE2  | 1:43:A:TYR:H    | 33       | 0.18          |
| (1,1904) | 1:66:A:MET:HE3  | 1:43:A:TYR:H    | 33       | 0.18          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1853) | 1:27:A:ALA:HB1 | 1:28:A:THR:H   | 25       | 0.18          |
| (1,1853) | 1:27:A:ALA:HB2 | 1:28:A:THR:H   | 25       | 0.18          |
| (1,1853) | 1:27:A:ALA:HB3 | 1:28:A:THR:H   | 25       | 0.18          |
| (1,1853) | 1:27:A:ALA:HB1 | 1:28:A:THR:H   | 29       | 0.18          |
| (1,1853) | 1:27:A:ALA:HB2 | 1:28:A:THR:H   | 29       | 0.18          |
| (1,1853) | 1:27:A:ALA:HB3 | 1:28:A:THR:H   | 29       | 0.18          |
| (1,1853) | 1:27:A:ALA:HB1 | 1:28:A:THR:H   | 30       | 0.18          |
| (1,1853) | 1:27:A:ALA:HB2 | 1:28:A:THR:H   | 30       | 0.18          |
| (1,1853) | 1:27:A:ALA:HB3 | 1:28:A:THR:H   | 30       | 0.18          |
| (1,1853) | 1:27:A:ALA:HB1 | 1:28:A:THR:H   | 31       | 0.18          |
| (1,1853) | 1:27:A:ALA:HB2 | 1:28:A:THR:H   | 31       | 0.18          |
| (1,1853) | 1:27:A:ALA:HB3 | 1:28:A:THR:H   | 31       | 0.18          |
| (1,1853) | 1:27:A:ALA:HB1 | 1:28:A:THR:H   | 32       | 0.18          |
| (1,1853) | 1:27:A:ALA:HB2 | 1:28:A:THR:H   | 32       | 0.18          |
| (1,1853) | 1:27:A:ALA:HB3 | 1:28:A:THR:H   | 32       | 0.18          |
| (1,1825) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 27       | 0.18          |
| (1,1825) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 29       | 0.18          |
| (1,1812) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 27       | 0.18          |
| (1,1812) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HA  | 29       | 0.18          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 3        | 0.18          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 5        | 0.18          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 6        | 0.18          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 7        | 0.18          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 8        | 0.18          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 14       | 0.18          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 15       | 0.18          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 16       | 0.18          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 17       | 0.18          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 19       | 0.18          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 24       | 0.18          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 26       | 0.18          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 35       | 0.18          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 37       | 0.18          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 40       | 0.18          |
| (1,1778) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 22       | 0.18          |
| (1,1778) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 23       | 0.18          |
| (1,1778) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 24       | 0.18          |
| (1,1778) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 28       | 0.18          |
| (1,1778) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 32       | 0.18          |
| (1,1778) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 34       | 0.18          |
| (1,1778) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 35       | 0.18          |
| (1,1744) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H   | 2        | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1744) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 11       | 0.18          |
| (1,1744) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 17       | 0.18          |
| (1,1744) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 18       | 0.18          |
| (1,1744) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 21       | 0.18          |
| (1,1744) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 22       | 0.18          |
| (1,1744) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 24       | 0.18          |
| (1,1744) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 27       | 0.18          |
| (1,1744) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 30       | 0.18          |
| (1,1744) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 39       | 0.18          |
| (1,1728) | 1:48:A:GLU:HB2  | 1:48:A:GLU:H    | 1        | 0.18          |
| (1,1728) | 1:48:A:GLU:HB2  | 1:48:A:GLU:H    | 3        | 0.18          |
| (1,1728) | 1:48:A:GLU:HB2  | 1:48:A:GLU:H    | 8        | 0.18          |
| (1,1728) | 1:48:A:GLU:HB2  | 1:48:A:GLU:H    | 14       | 0.18          |
| (1,1728) | 1:48:A:GLU:HB2  | 1:48:A:GLU:H    | 22       | 0.18          |
| (1,1728) | 1:48:A:GLU:HB2  | 1:48:A:GLU:H    | 27       | 0.18          |
| (1,1728) | 1:48:A:GLU:HB2  | 1:48:A:GLU:H    | 32       | 0.18          |
| (1,1728) | 1:48:A:GLU:HB2  | 1:48:A:GLU:H    | 33       | 0.18          |
| (1,1728) | 1:48:A:GLU:HB2  | 1:48:A:GLU:H    | 38       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 11       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 11       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 11       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 11       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 11       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 11       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 11       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 11       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 11       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 22       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 22       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 22       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 22       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 22       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 22       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 22       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 22       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 22       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 25       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 25       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 25       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 25       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 25       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 25       | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 25       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 25       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 25       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 34       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 34       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 34       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 34       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 34       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 34       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 34       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 34       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 34       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 39       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 39       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 39       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 39       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 39       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 39       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 39       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 39       | 0.18          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 39       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 10       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 10       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 10       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 10       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 10       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 10       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 10       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 10       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 10       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 22       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 22       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 22       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 22       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 22       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 22       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 22       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 22       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 22       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 23       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 23       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 23       | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 23       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 23       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 23       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 23       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 23       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 23       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 25       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 25       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 25       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 25       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 25       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 25       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 25       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 25       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 25       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 30       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 30       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 30       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 30       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 30       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 30       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 30       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 30       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 30       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 34       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 34       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 34       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 34       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 34       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 34       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 34       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 34       | 0.18          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 34       | 0.18          |
| (1,1624) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2  | 38       | 0.18          |
| (1,1624) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2  | 38       | 0.18          |
| (1,1624) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2  | 38       | 0.18          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 1        | 0.18          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 1        | 0.18          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 1        | 0.18          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 3        | 0.18          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 3        | 0.18          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 3        | 0.18          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 4        | 0.18          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 4        | 0.18          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 4        | 0.18          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 5        | 0.18          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 5        | 0.18          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 5        | 0.18          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 6        | 0.18          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 6        | 0.18          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 6        | 0.18          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 7        | 0.18          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 7        | 0.18          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 7        | 0.18          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 9        | 0.18          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 9        | 0.18          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 9        | 0.18          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 10       | 0.18          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 10       | 0.18          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 10       | 0.18          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 26       | 0.18          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 26       | 0.18          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 26       | 0.18          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 28       | 0.18          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 28       | 0.18          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 28       | 0.18          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 31       | 0.18          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 31       | 0.18          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 31       | 0.18          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 35       | 0.18          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 35       | 0.18          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 35       | 0.18          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 36       | 0.18          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 36       | 0.18          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 36       | 0.18          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 38       | 0.18          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 38       | 0.18          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 38       | 0.18          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2 | 5        | 0.18          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 5        | 0.18          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 5        | 0.18          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2 | 8        | 0.18          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 8        | 0.18          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 8        | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 18       | 0.18          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 18       | 0.18          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 18       | 0.18          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 40       | 0.18          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 40       | 0.18          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 40       | 0.18          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1  | 1        | 0.18          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2  | 1        | 0.18          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1  | 1        | 0.18          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2  | 1        | 0.18          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1  | 1        | 0.18          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2  | 1        | 0.18          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 16       | 0.18          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 16       | 0.18          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 16       | 0.18          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 16       | 0.18          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 16       | 0.18          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 16       | 0.18          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 3        | 0.18          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 3        | 0.18          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 3        | 0.18          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 8        | 0.18          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 8        | 0.18          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 8        | 0.18          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 22       | 0.18          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 22       | 0.18          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 22       | 0.18          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 26       | 0.18          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 26       | 0.18          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 26       | 0.18          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 31       | 0.18          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 31       | 0.18          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 31       | 0.18          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 36       | 0.18          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 36       | 0.18          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 36       | 0.18          |
| (1,1578) | 1:39:A:ILE:HG21 | 1:39:A:ILE:HG12 | 3        | 0.18          |
| (1,1578) | 1:39:A:ILE:HG22 | 1:39:A:ILE:HG12 | 3        | 0.18          |
| (1,1578) | 1:39:A:ILE:HG23 | 1:39:A:ILE:HG12 | 3        | 0.18          |
| (1,1543) | 1:2:A:ILE:HG12  | 1:2:A:ILE:HA    | 23       | 0.18          |
| (1,1530) | 1:2:A:ILE:HG21  | 1:2:A:ILE:HA    | 10       | 0.18          |
| (1,1530) | 1:2:A:ILE:HG22  | 1:2:A:ILE:HA    | 10       | 0.18          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1530) | 1:2:A:ILE:HG23  | 1:2:A:ILE:HA   | 10       | 0.18          |
| (1,1530) | 1:2:A:ILE:HG21  | 1:2:A:ILE:HA   | 14       | 0.18          |
| (1,1530) | 1:2:A:ILE:HG22  | 1:2:A:ILE:HA   | 14       | 0.18          |
| (1,1530) | 1:2:A:ILE:HG23  | 1:2:A:ILE:HA   | 14       | 0.18          |
| (1,1530) | 1:2:A:ILE:HG21  | 1:2:A:ILE:HA   | 17       | 0.18          |
| (1,1530) | 1:2:A:ILE:HG22  | 1:2:A:ILE:HA   | 17       | 0.18          |
| (1,1530) | 1:2:A:ILE:HG23  | 1:2:A:ILE:HA   | 17       | 0.18          |
| (1,1530) | 1:2:A:ILE:HG21  | 1:2:A:ILE:HA   | 23       | 0.18          |
| (1,1530) | 1:2:A:ILE:HG22  | 1:2:A:ILE:HA   | 23       | 0.18          |
| (1,1530) | 1:2:A:ILE:HG23  | 1:2:A:ILE:HA   | 23       | 0.18          |
| (1,1530) | 1:2:A:ILE:HG21  | 1:2:A:ILE:HA   | 37       | 0.18          |
| (1,1530) | 1:2:A:ILE:HG22  | 1:2:A:ILE:HA   | 37       | 0.18          |
| (1,1530) | 1:2:A:ILE:HG23  | 1:2:A:ILE:HA   | 37       | 0.18          |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1 | 3        | 0.18          |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2 | 3        | 0.18          |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1 | 3        | 0.18          |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2 | 3        | 0.18          |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1 | 3        | 0.18          |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2 | 3        | 0.18          |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1 | 14       | 0.18          |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2 | 14       | 0.18          |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1 | 14       | 0.18          |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2 | 14       | 0.18          |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1 | 14       | 0.18          |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2 | 14       | 0.18          |
| (1,1508) | 1:66:A:MET:HE1  | 1:42:A:TRP:HZ3 | 11       | 0.18          |
| (1,1508) | 1:66:A:MET:HE2  | 1:42:A:TRP:HZ3 | 11       | 0.18          |
| (1,1508) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3 | 11       | 0.18          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 2        | 0.18          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 2        | 0.18          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 2        | 0.18          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 5        | 0.18          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 5        | 0.18          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 5        | 0.18          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 38       | 0.18          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 38       | 0.18          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 38       | 0.18          |
| (1,1475) | 1:78:A:VAL:HG11 | 1:94:A:THR:HA  | 28       | 0.18          |
| (1,1475) | 1:78:A:VAL:HG12 | 1:94:A:THR:HA  | 28       | 0.18          |
| (1,1475) | 1:78:A:VAL:HG13 | 1:94:A:THR:HA  | 28       | 0.18          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 1        | 0.18          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 1        | 0.18          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 1        | 0.18          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 2        | 0.18          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 2        | 0.18          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 2        | 0.18          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 3        | 0.18          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 3        | 0.18          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 3        | 0.18          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 22       | 0.18          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 22       | 0.18          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 22       | 0.18          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 27       | 0.18          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 27       | 0.18          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 27       | 0.18          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 38       | 0.18          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 38       | 0.18          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 38       | 0.18          |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 2        | 0.18          |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 2        | 0.18          |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 2        | 0.18          |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 14       | 0.18          |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 14       | 0.18          |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 14       | 0.18          |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 20       | 0.18          |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 20       | 0.18          |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 20       | 0.18          |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 35       | 0.18          |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 35       | 0.18          |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 35       | 0.18          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 4        | 0.18          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 4        | 0.18          |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 4        | 0.18          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 20       | 0.18          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 20       | 0.18          |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 20       | 0.18          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 24       | 0.18          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 24       | 0.18          |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 24       | 0.18          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 28       | 0.18          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 28       | 0.18          |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 28       | 0.18          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 33       | 0.18          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 33       | 0.18          |

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| Key      | Atom-1          | Atom-2       | Model ID | Violation (Å) |
|----------|-----------------|--------------|----------|---------------|
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H | 33       | 0.18          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H | 34       | 0.18          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H | 34       | 0.18          |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H | 34       | 0.18          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 8        | 0.18          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 8        | 0.18          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 8        | 0.18          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 12       | 0.18          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 12       | 0.18          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 12       | 0.18          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 13       | 0.18          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 13       | 0.18          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 13       | 0.18          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 24       | 0.18          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 24       | 0.18          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 24       | 0.18          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 31       | 0.18          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 31       | 0.18          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 31       | 0.18          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 38       | 0.18          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 38       | 0.18          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 38       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 7        | 0.18          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 7        | 0.18          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 7        | 0.18          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 11       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 11       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 11       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 14       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 14       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 14       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 16       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 16       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 16       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 18       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 18       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 18       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 19       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 19       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 19       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 21       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 21       | 0.18          |

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| Key      | Atom-1          | Atom-2       | Model ID | Violation (Å) |
|----------|-----------------|--------------|----------|---------------|
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 21       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 22       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 22       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 22       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 24       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 24       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 24       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 25       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 25       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 25       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 26       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 26       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 26       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 27       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 27       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 27       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 30       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 30       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 30       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 31       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 31       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 31       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 33       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 33       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 33       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 35       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 35       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 35       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 36       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 36       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 36       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 37       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 37       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 37       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 38       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 38       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 38       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 40       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 40       | 0.18          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 40       | 0.18          |
| (1,1401) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H | 6        | 0.18          |
| (1,1401) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H | 6        | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1401) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H    | 6        | 0.18          |
| (1,1401) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H    | 37       | 0.18          |
| (1,1401) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H    | 37       | 0.18          |
| (1,1401) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H    | 37       | 0.18          |
| (1,1396) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA   | 2        | 0.18          |
| (1,1396) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA   | 2        | 0.18          |
| (1,1396) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA   | 2        | 0.18          |
| (1,1396) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA   | 15       | 0.18          |
| (1,1396) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA   | 15       | 0.18          |
| (1,1396) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA   | 15       | 0.18          |
| (1,1396) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA   | 22       | 0.18          |
| (1,1396) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA   | 22       | 0.18          |
| (1,1396) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA   | 22       | 0.18          |
| (1,1387) | 1:91:A:ALA:HB1  | 1:12:A:PHE:HZ   | 20       | 0.18          |
| (1,1387) | 1:91:A:ALA:HB2  | 1:12:A:PHE:HZ   | 20       | 0.18          |
| (1,1387) | 1:91:A:ALA:HB3  | 1:12:A:PHE:HZ   | 20       | 0.18          |
| (1,1387) | 1:91:A:ALA:HB1  | 1:12:A:PHE:HZ   | 38       | 0.18          |
| (1,1387) | 1:91:A:ALA:HB2  | 1:12:A:PHE:HZ   | 38       | 0.18          |
| (1,1387) | 1:91:A:ALA:HB3  | 1:12:A:PHE:HZ   | 38       | 0.18          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 8        | 0.18          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 23       | 0.18          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 25       | 0.18          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 9        | 0.18          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 9        | 0.18          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 9        | 0.18          |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H    | 28       | 0.18          |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H    | 28       | 0.18          |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H    | 28       | 0.18          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 13       | 0.18          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 13       | 0.18          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 13       | 0.18          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 13       | 0.18          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 13       | 0.18          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 13       | 0.18          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 13       | 0.18          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 13       | 0.18          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 13       | 0.18          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 20       | 0.18          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 20       | 0.18          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 20       | 0.18          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 20       | 0.18          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 20       | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 20       | 0.18          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 20       | 0.18          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 20       | 0.18          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 20       | 0.18          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 4        | 0.18          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 4        | 0.18          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 4        | 0.18          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 5        | 0.18          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 5        | 0.18          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 5        | 0.18          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 11       | 0.18          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 11       | 0.18          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 11       | 0.18          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 13       | 0.18          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 13       | 0.18          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 13       | 0.18          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 31       | 0.18          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 31       | 0.18          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 31       | 0.18          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 4        | 0.18          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 4        | 0.18          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 4        | 0.18          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 5        | 0.18          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 5        | 0.18          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 5        | 0.18          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 11       | 0.18          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 11       | 0.18          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 11       | 0.18          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 13       | 0.18          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 13       | 0.18          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 13       | 0.18          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 31       | 0.18          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 31       | 0.18          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 31       | 0.18          |
| (1,1257) | 1:67:A:THR:HG21 | 1:26:A:SER:HB2  | 6        | 0.18          |
| (1,1257) | 1:67:A:THR:HG22 | 1:26:A:SER:HB2  | 6        | 0.18          |
| (1,1257) | 1:67:A:THR:HG23 | 1:26:A:SER:HB2  | 6        | 0.18          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 3        | 0.18          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 3        | 0.18          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 3        | 0.18          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 13       | 0.18          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 13       | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 13       | 0.18          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 18       | 0.18          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 18       | 0.18          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 18       | 0.18          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 5        | 0.18          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 5        | 0.18          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 5        | 0.18          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 31       | 0.18          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 31       | 0.18          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 31       | 0.18          |
| (1,1236) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3  | 28       | 0.18          |
| (1,1236) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3  | 28       | 0.18          |
| (1,1236) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3  | 28       | 0.18          |
| (1,1213) | 1:66:A:MET:H    | 1:28:A:THR:HA   | 10       | 0.18          |
| (1,1213) | 1:66:A:MET:H    | 1:28:A:THR:HA   | 26       | 0.18          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 1        | 0.18          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 1        | 0.18          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 1        | 0.18          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 2        | 0.18          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 2        | 0.18          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 2        | 0.18          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 12       | 0.18          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 12       | 0.18          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 12       | 0.18          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 13       | 0.18          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 13       | 0.18          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 13       | 0.18          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 26       | 0.18          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 26       | 0.18          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 26       | 0.18          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 28       | 0.18          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 28       | 0.18          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 28       | 0.18          |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 2        | 0.18          |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 6        | 0.18          |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 13       | 0.18          |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 33       | 0.18          |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 34       | 0.18          |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 23       | 0.18          |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 27       | 0.18          |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 32       | 0.18          |
| (1,1169) | 1:14:A:LYS:H    | 1:14:A:LYS:HD2  | 37       | 0.18          |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1163) | 1:75:A:ASP:H  | 1:74:A:ASP:HB2  | 29       | 0.18          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 12       | 0.18          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 12       | 0.18          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 24       | 0.18          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 24       | 0.18          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 29       | 0.18          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 29       | 0.18          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 35       | 0.18          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 35       | 0.18          |
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 5        | 0.18          |
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 7        | 0.18          |
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 11       | 0.18          |
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 13       | 0.18          |
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 26       | 0.18          |
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 27       | 0.18          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 1        | 0.18          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 2        | 0.18          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 4        | 0.18          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 9        | 0.18          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 16       | 0.18          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 20       | 0.18          |
| (1,1020) | 1:48:A:GLU:H  | 1:48:A:GLU:HG3  | 37       | 0.18          |
| (1,962)  | 1:102:A:ARG:H | 1:101:A:LEU:HB2 | 23       | 0.18          |
| (1,941)  | 1:34:A:SER:H  | 1:12:A:PHE:HA   | 28       | 0.18          |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 3        | 0.18          |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 7        | 0.18          |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 10       | 0.18          |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 12       | 0.18          |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 16       | 0.18          |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 22       | 0.18          |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 23       | 0.18          |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 26       | 0.18          |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 28       | 0.18          |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 31       | 0.18          |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 32       | 0.18          |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 36       | 0.18          |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 40       | 0.18          |
| (1,918)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB3  | 24       | 0.18          |
| (1,918)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB3  | 38       | 0.18          |
| (1,888)  | 1:80:A:SER:H  | 1:43:A:TYR:HB3  | 18       | 0.18          |
| (1,888)  | 1:80:A:SER:H  | 1:43:A:TYR:HB3  | 34       | 0.18          |
| (1,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3   | 1        | 0.18          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3   | 3        | 0.18          |
| (1,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3   | 4        | 0.18          |
| (1,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3   | 14       | 0.18          |
| (1,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3   | 17       | 0.18          |
| (1,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3   | 19       | 0.18          |
| (1,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3   | 33       | 0.18          |
| (1,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2   | 22       | 0.18          |
| (1,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2   | 27       | 0.18          |
| (1,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2   | 35       | 0.18          |
| (1,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2   | 38       | 0.18          |
| (1,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 1        | 0.18          |
| (1,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 3        | 0.18          |
| (1,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 15       | 0.18          |
| (1,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 18       | 0.18          |
| (1,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 24       | 0.18          |
| (1,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 38       | 0.18          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 37       | 0.18          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 37       | 0.18          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 37       | 0.18          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 7        | 0.18          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 4        | 0.18          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 4        | 0.18          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 4        | 0.18          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 13       | 0.18          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 13       | 0.18          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 13       | 0.18          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 35       | 0.18          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 35       | 0.18          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 35       | 0.18          |
| (1,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB   | 8        | 0.18          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 1        | 0.18          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 6        | 0.18          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 8        | 0.18          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 14       | 0.18          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 39       | 0.18          |
| (1,786) | 1:6:A:THR:H  | 1:6:A:THR:HG21  | 6        | 0.18          |
| (1,786) | 1:6:A:THR:H  | 1:6:A:THR:HG22  | 6        | 0.18          |
| (1,786) | 1:6:A:THR:H  | 1:6:A:THR:HG23  | 6        | 0.18          |
| (1,783) | 1:74:A:ASP:H | 1:74:A:ASP:HB3  | 36       | 0.18          |
| (1,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2  | 1        | 0.18          |
| (1,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2  | 6        | 0.18          |
| (1,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2  | 23       | 0.18          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 3        | 0.18          |
| (1,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 20       | 0.18          |
| (1,737) | 1:15:A:ARG:H  | 1:14:A:LYS:HA   | 40       | 0.18          |
| (1,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 20       | 0.18          |
| (1,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 9        | 0.18          |
| (1,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 12       | 0.18          |
| (1,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 27       | 0.18          |
| (1,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 28       | 0.18          |
| (1,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 38       | 0.18          |
| (1,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3  | 22       | 0.18          |
| (1,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3  | 33       | 0.18          |
| (1,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3  | 34       | 0.18          |
| (1,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3  | 35       | 0.18          |
| (1,715) | 1:16:A:ILE:H  | 1:15:A:ARG:HB3  | 37       | 0.18          |
| (1,684) | 1:23:A:GLU:H  | 1:23:A:GLU:HB3  | 24       | 0.18          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 2        | 0.18          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 22       | 0.18          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 9        | 0.18          |
| (1,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 3        | 0.18          |
| (1,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 9        | 0.18          |
| (1,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 18       | 0.18          |
| (1,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 26       | 0.18          |
| (1,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 30       | 0.18          |
| (1,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 38       | 0.18          |
| (1,560) | 1:47:A:THR:H  | 1:47:A:THR:HA   | 1        | 0.18          |
| (1,560) | 1:47:A:THR:H  | 1:47:A:THR:HA   | 7        | 0.18          |
| (1,560) | 1:47:A:THR:H  | 1:47:A:THR:HA   | 12       | 0.18          |
| (1,560) | 1:47:A:THR:H  | 1:47:A:THR:HA   | 17       | 0.18          |
| (1,560) | 1:47:A:THR:H  | 1:47:A:THR:HA   | 29       | 0.18          |
| (1,560) | 1:47:A:THR:H  | 1:47:A:THR:HA   | 30       | 0.18          |
| (1,560) | 1:47:A:THR:H  | 1:47:A:THR:HA   | 37       | 0.18          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 9        | 0.18          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2  | 9        | 0.18          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 11       | 0.18          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2  | 11       | 0.18          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 14       | 0.18          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2  | 14       | 0.18          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 15       | 0.18          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2  | 15       | 0.18          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 39       | 0.18          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2  | 39       | 0.18          |
| (1,546) | 1:71:A:VAL:H  | 1:24:A:HIS:HA   | 3        | 0.18          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 26       | 0.18          |
| (1,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 34       | 0.18          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 1        | 0.18          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 2        | 0.18          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 5        | 0.18          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 8        | 0.18          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 20       | 0.18          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 21       | 0.18          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 24       | 0.18          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 27       | 0.18          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 28       | 0.18          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 31       | 0.18          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 9        | 0.18          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 15       | 0.18          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 21       | 0.18          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 8        | 0.18          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 11       | 0.18          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 13       | 0.18          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 21       | 0.18          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 23       | 0.18          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 25       | 0.18          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 26       | 0.18          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 30       | 0.18          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 35       | 0.18          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 36       | 0.18          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 3        | 0.18          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 8        | 0.18          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 14       | 0.18          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 20       | 0.18          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 35       | 0.18          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 37       | 0.18          |
| (1,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 3        | 0.18          |
| (1,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 22       | 0.18          |
| (1,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 23       | 0.18          |
| (1,410) | 1:96:A:GLU:H | 1:18:A:ASN:HD21 | 29       | 0.18          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 8        | 0.18          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 17       | 0.18          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 24       | 0.18          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 29       | 0.18          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 30       | 0.18          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 32       | 0.18          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 33       | 0.18          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 40       | 0.18          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 27       | 0.18          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 27       | 0.18          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 27       | 0.18          |
| (1,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 18       | 0.18          |
| (1,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 29       | 0.18          |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 31       | 0.18          |
| (1,274) | 1:66:A:MET:H | 1:66:A:MET:HG3  | 7        | 0.18          |
| (1,274) | 1:66:A:MET:H | 1:66:A:MET:HG3  | 15       | 0.18          |
| (1,274) | 1:66:A:MET:H | 1:66:A:MET:HG3  | 24       | 0.18          |
| (1,274) | 1:66:A:MET:H | 1:66:A:MET:HG3  | 29       | 0.18          |
| (1,274) | 1:66:A:MET:H | 1:66:A:MET:HG3  | 33       | 0.18          |
| (1,274) | 1:66:A:MET:H | 1:66:A:MET:HG3  | 39       | 0.18          |
| (1,274) | 1:66:A:MET:H | 1:66:A:MET:HG3  | 40       | 0.18          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 4        | 0.18          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 4        | 0.18          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 4        | 0.18          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 5        | 0.18          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 5        | 0.18          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 5        | 0.18          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 11       | 0.18          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 11       | 0.18          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 11       | 0.18          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 13       | 0.18          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 13       | 0.18          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 13       | 0.18          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 31       | 0.18          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 31       | 0.18          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 31       | 0.18          |
| (1,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 2        | 0.18          |
| (1,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 3        | 0.18          |
| (1,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 5        | 0.18          |
| (1,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 6        | 0.18          |
| (1,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 8        | 0.18          |
| (1,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 10       | 0.18          |
| (1,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 12       | 0.18          |
| (1,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 14       | 0.18          |
| (1,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 16       | 0.18          |
| (1,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 19       | 0.18          |
| (1,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 21       | 0.18          |
| (1,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 22       | 0.18          |
| (1,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 24       | 0.18          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 27       | 0.18          |
| (1,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 28       | 0.18          |
| (1,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 31       | 0.18          |
| (1,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 33       | 0.18          |
| (1,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 35       | 0.18          |
| (1,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 36       | 0.18          |
| (1,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 38       | 0.18          |
| (1,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 39       | 0.18          |
| (1,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 1        | 0.18          |
| (1,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 37       | 0.18          |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG21 | 12       | 0.18          |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG22 | 12       | 0.18          |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG23 | 12       | 0.18          |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG21 | 28       | 0.18          |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG22 | 28       | 0.18          |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG23 | 28       | 0.18          |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG21 | 35       | 0.18          |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG22 | 35       | 0.18          |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG23 | 35       | 0.18          |
| (1,149) | 1:45:A:GLY:H  | 1:46:A:PRO:HD3  | 9        | 0.18          |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 5        | 0.18          |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 7        | 0.18          |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 11       | 0.18          |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 13       | 0.18          |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 26       | 0.18          |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 27       | 0.18          |
| (1,133) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 6        | 0.18          |
| (1,133) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 9        | 0.18          |
| (1,133) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 21       | 0.18          |
| (1,133) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 39       | 0.18          |
| (1,129) | 1:39:A:ILE:H  | 1:39:A:ILE:HA   | 2        | 0.18          |
| (1,129) | 1:39:A:ILE:H  | 1:39:A:ILE:HA   | 11       | 0.18          |
| (1,100) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 1        | 0.18          |
| (1,100) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 2        | 0.18          |
| (1,100) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 10       | 0.18          |
| (1,100) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 13       | 0.18          |
| (1,100) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 17       | 0.18          |
| (1,100) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 18       | 0.18          |
| (1,100) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 21       | 0.18          |
| (1,100) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 22       | 0.18          |
| (1,100) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 23       | 0.18          |
| (1,100) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 25       | 0.18          |

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| Key      | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|----------|---------------|----------------|----------|---------------|
| (1,100)  | 1:22:A:SER:H  | 1:21:A:VAL:HB  | 26       | 0.18          |
| (1,100)  | 1:22:A:SER:H  | 1:21:A:VAL:HB  | 27       | 0.18          |
| (1,100)  | 1:22:A:SER:H  | 1:21:A:VAL:HB  | 28       | 0.18          |
| (1,100)  | 1:22:A:SER:H  | 1:21:A:VAL:HB  | 30       | 0.18          |
| (1,100)  | 1:22:A:SER:H  | 1:21:A:VAL:HB  | 33       | 0.18          |
| (1,100)  | 1:22:A:SER:H  | 1:21:A:VAL:HB  | 36       | 0.18          |
| (1,100)  | 1:22:A:SER:H  | 1:21:A:VAL:HB  | 40       | 0.18          |
| (1,70)   | 1:51:A:GLU:H  | 1:51:A:GLU:HG2 | 2        | 0.18          |
| (1,70)   | 1:51:A:GLU:H  | 1:51:A:GLU:HG2 | 11       | 0.18          |
| (1,70)   | 1:51:A:GLU:H  | 1:51:A:GLU:HG2 | 17       | 0.18          |
| (1,70)   | 1:51:A:GLU:H  | 1:51:A:GLU:HG2 | 18       | 0.18          |
| (1,70)   | 1:51:A:GLU:H  | 1:51:A:GLU:HG2 | 21       | 0.18          |
| (1,70)   | 1:51:A:GLU:H  | 1:51:A:GLU:HG2 | 22       | 0.18          |
| (1,70)   | 1:51:A:GLU:H  | 1:51:A:GLU:HG2 | 24       | 0.18          |
| (1,70)   | 1:51:A:GLU:H  | 1:51:A:GLU:HG2 | 27       | 0.18          |
| (1,70)   | 1:51:A:GLU:H  | 1:51:A:GLU:HG2 | 30       | 0.18          |
| (1,70)   | 1:51:A:GLU:H  | 1:51:A:GLU:HG2 | 39       | 0.18          |
| (1,57)   | 1:42:A:TRP:H  | 1:41:A:THR:HB  | 1        | 0.18          |
| (1,57)   | 1:42:A:TRP:H  | 1:41:A:THR:HB  | 3        | 0.18          |
| (1,57)   | 1:42:A:TRP:H  | 1:41:A:THR:HB  | 8        | 0.18          |
| (1,57)   | 1:42:A:TRP:H  | 1:41:A:THR:HB  | 15       | 0.18          |
| (1,57)   | 1:42:A:TRP:H  | 1:41:A:THR:HB  | 27       | 0.18          |
| (1,49)   | 1:57:A:PHE:H  | 1:56:A:ASN:HB2 | 2        | 0.18          |
| (1,49)   | 1:57:A:PHE:H  | 1:56:A:ASN:HB2 | 5        | 0.18          |
| (1,49)   | 1:57:A:PHE:H  | 1:56:A:ASN:HB2 | 9        | 0.18          |
| (1,49)   | 1:57:A:PHE:H  | 1:56:A:ASN:HB2 | 11       | 0.18          |
| (1,49)   | 1:57:A:PHE:H  | 1:56:A:ASN:HB2 | 13       | 0.18          |
| (1,49)   | 1:57:A:PHE:H  | 1:56:A:ASN:HB2 | 21       | 0.18          |
| (1,49)   | 1:57:A:PHE:H  | 1:56:A:ASN:HB2 | 23       | 0.18          |
| (1,49)   | 1:57:A:PHE:H  | 1:56:A:ASN:HB2 | 29       | 0.18          |
| (1,49)   | 1:57:A:PHE:H  | 1:56:A:ASN:HB2 | 32       | 0.18          |
| (1,49)   | 1:57:A:PHE:H  | 1:56:A:ASN:HB2 | 33       | 0.18          |
| (1,49)   | 1:57:A:PHE:H  | 1:56:A:ASN:HB2 | 37       | 0.18          |
| (1,49)   | 1:57:A:PHE:H  | 1:56:A:ASN:HB2 | 38       | 0.18          |
| (1,49)   | 1:57:A:PHE:H  | 1:56:A:ASN:HB2 | 39       | 0.18          |
| (3,3215) | 1:57:A:PHE:HZ | 1:55:A:TYR:HD1 | 4        | 0.17          |
| (3,3215) | 1:57:A:PHE:HZ | 1:55:A:TYR:HD2 | 4        | 0.17          |
| (3,3215) | 1:57:A:PHE:HZ | 1:55:A:TYR:HD1 | 6        | 0.17          |
| (3,3215) | 1:57:A:PHE:HZ | 1:55:A:TYR:HD2 | 6        | 0.17          |
| (3,3215) | 1:57:A:PHE:HZ | 1:55:A:TYR:HD1 | 10       | 0.17          |
| (3,3215) | 1:57:A:PHE:HZ | 1:55:A:TYR:HD2 | 10       | 0.17          |
| (3,3215) | 1:57:A:PHE:HZ | 1:55:A:TYR:HD1 | 15       | 0.17          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 15       | 0.17          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 16       | 0.17          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 16       | 0.17          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 40       | 0.17          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 40       | 0.17          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 1        | 0.17          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 1        | 0.17          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 1        | 0.17          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 1        | 0.17          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 1        | 0.17          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 1        | 0.17          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 19       | 0.17          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 19       | 0.17          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 19       | 0.17          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 19       | 0.17          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 19       | 0.17          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 19       | 0.17          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 20       | 0.17          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 20       | 0.17          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 20       | 0.17          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 20       | 0.17          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 20       | 0.17          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 20       | 0.17          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 30       | 0.17          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 30       | 0.17          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 30       | 0.17          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 30       | 0.17          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 30       | 0.17          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 30       | 0.17          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 33       | 0.17          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 33       | 0.17          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 33       | 0.17          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 33       | 0.17          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 33       | 0.17          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 33       | 0.17          |
| (3,3205) | 1:43:A:TYR:HD1 | 1:80:A:SER:HB2  | 21       | 0.17          |
| (3,3205) | 1:43:A:TYR:HD2 | 1:80:A:SER:HB2  | 21       | 0.17          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 1        | 0.17          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 2        | 0.17          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 21       | 0.17          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 22       | 0.17          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 30       | 0.17          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 33       | 0.17          |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2  | 36       | 0.17          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2  | 36       | 0.17          |
| (3,3138) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB2  | 5        | 0.17          |
| (3,3138) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB2  | 5        | 0.17          |
| (3,3137) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3  | 17       | 0.17          |
| (3,3137) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3  | 17       | 0.17          |
| (3,3137) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3  | 34       | 0.17          |
| (3,3137) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3  | 34       | 0.17          |
| (3,3133) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 22       | 0.17          |
| (3,3133) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 22       | 0.17          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 3        | 0.17          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 3        | 0.17          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 9        | 0.17          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 9        | 0.17          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 11       | 0.17          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 11       | 0.17          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 18       | 0.17          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 18       | 0.17          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 26       | 0.17          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 26       | 0.17          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 29       | 0.17          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 29       | 0.17          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 3        | 0.17          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 3        | 0.17          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 9        | 0.17          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 9        | 0.17          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 11       | 0.17          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 11       | 0.17          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 18       | 0.17          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 18       | 0.17          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 26       | 0.17          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 26       | 0.17          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 29       | 0.17          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 29       | 0.17          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 20       | 0.17          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 20       | 0.17          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 20       | 0.17          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 20       | 0.17          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 20       | 0.17          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 20       | 0.17          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 28       | 0.17          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 28       | 0.17          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 28       | 0.17          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 28       | 0.17          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 28       | 0.17          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 28       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 1        | 0.17          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 1        | 0.17          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 1        | 0.17          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 1        | 0.17          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 1        | 0.17          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 1        | 0.17          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 20       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 20       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 20       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 20       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 20       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 20       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 26       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 26       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 26       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 26       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 26       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 26       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 32       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 32       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 32       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 32       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 32       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 32       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 35       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 35       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 35       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 35       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 35       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 35       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 37       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 37       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 37       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 37       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 37       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 37       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 38       | 0.17          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 38       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 38       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 38       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 38       | 0.17          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 38       | 0.17          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 1        | 0.17          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 1        | 0.17          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 1        | 0.17          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 1        | 0.17          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 7        | 0.17          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 7        | 0.17          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 7        | 0.17          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 7        | 0.17          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 11       | 0.17          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 11       | 0.17          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 11       | 0.17          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 11       | 0.17          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 16       | 0.17          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 16       | 0.17          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 16       | 0.17          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 16       | 0.17          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 17       | 0.17          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 17       | 0.17          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 17       | 0.17          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 17       | 0.17          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 12       | 0.17          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 12       | 0.17          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 12       | 0.17          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 12       | 0.17          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 12       | 0.17          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 12       | 0.17          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 21       | 0.17          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 21       | 0.17          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 21       | 0.17          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 21       | 0.17          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 21       | 0.17          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 21       | 0.17          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 1        | 0.17          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 2        | 0.17          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 3        | 0.17          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 4        | 0.17          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 5        | 0.17          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 6        | 0.17          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 11       | 0.17          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 14       | 0.17          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 15       | 0.17          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 17       | 0.17          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 29       | 0.17          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 33       | 0.17          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 34       | 0.17          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 37       | 0.17          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 13       | 0.17          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 13       | 0.17          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 13       | 0.17          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 18       | 0.17          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 18       | 0.17          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 18       | 0.17          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 27       | 0.17          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 27       | 0.17          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 27       | 0.17          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 13       | 0.17          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 13       | 0.17          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 35       | 0.17          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 35       | 0.17          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 14       | 0.17          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 27       | 0.17          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 28       | 0.17          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 31       | 0.17          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 38       | 0.17          |
| (3,3041) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE1  | 15       | 0.17          |
| (3,3041) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE2  | 15       | 0.17          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 1        | 0.17          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 1        | 0.17          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 1        | 0.17          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 8        | 0.17          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 8        | 0.17          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 8        | 0.17          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 38       | 0.17          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 38       | 0.17          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 38       | 0.17          |
| (3,3004) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 6        | 0.17          |
| (3,3004) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 7        | 0.17          |
| (3,3004) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 12       | 0.17          |
| (3,3004) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 20       | 0.17          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,3004) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3 | 36       | 0.17          |
| (3,2982) | 1:65:A:TYR:HA  | 1:42:A:TRP:HZ2 | 8        | 0.17          |
| (3,2937) | 1:17:A:GLN:HG2 | 1:18:A:ASN:H   | 8        | 0.17          |
| (3,2925) | 1:22:A:SER:HB2 | 1:25:A:GLN:H   | 9        | 0.17          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 1        | 0.17          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 2        | 0.17          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 4        | 0.17          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 9        | 0.17          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 10       | 0.17          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 11       | 0.17          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 12       | 0.17          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 13       | 0.17          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 18       | 0.17          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 20       | 0.17          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 21       | 0.17          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 22       | 0.17          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 23       | 0.17          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 25       | 0.17          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 27       | 0.17          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 28       | 0.17          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 29       | 0.17          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 30       | 0.17          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 31       | 0.17          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 32       | 0.17          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 33       | 0.17          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 34       | 0.17          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 36       | 0.17          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 38       | 0.17          |
| (3,2914) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 39       | 0.17          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 1        | 0.17          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 2        | 0.17          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 4        | 0.17          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 9        | 0.17          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 10       | 0.17          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 11       | 0.17          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 12       | 0.17          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 13       | 0.17          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 18       | 0.17          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 20       | 0.17          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 21       | 0.17          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 22       | 0.17          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 23       | 0.17          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 25       | 0.17          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 27       | 0.17          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 28       | 0.17          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 29       | 0.17          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 30       | 0.17          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 31       | 0.17          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 32       | 0.17          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 33       | 0.17          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 34       | 0.17          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 36       | 0.17          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 38       | 0.17          |
| (3,2911) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 39       | 0.17          |
| (3,2910) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD2 | 18       | 0.17          |
| (3,2866) | 1:92:A:ARG:HB3 | 1:92:A:ARG:H   | 9        | 0.17          |
| (3,2866) | 1:92:A:ARG:HB3 | 1:92:A:ARG:H   | 10       | 0.17          |
| (3,2866) | 1:92:A:ARG:HB3 | 1:92:A:ARG:H   | 12       | 0.17          |
| (3,2866) | 1:92:A:ARG:HB3 | 1:92:A:ARG:H   | 20       | 0.17          |
| (3,2866) | 1:92:A:ARG:HB3 | 1:92:A:ARG:H   | 33       | 0.17          |
| (3,2761) | 1:90:A:GLU:HB3 | 1:91:A:ALA:H   | 6        | 0.17          |
| (3,2761) | 1:90:A:GLU:HB3 | 1:91:A:ALA:H   | 8        | 0.17          |
| (3,2761) | 1:90:A:GLU:HB3 | 1:91:A:ALA:H   | 12       | 0.17          |
| (3,2761) | 1:90:A:GLU:HB3 | 1:91:A:ALA:H   | 20       | 0.17          |
| (3,2761) | 1:90:A:GLU:HB3 | 1:91:A:ALA:H   | 36       | 0.17          |
| (3,2727) | 1:76:A:GLU:HB2 | 1:77:A:GLY:H   | 20       | 0.17          |
| (3,2727) | 1:76:A:GLU:HB2 | 1:77:A:GLY:H   | 27       | 0.17          |
| (3,2727) | 1:76:A:GLU:HB2 | 1:77:A:GLY:H   | 28       | 0.17          |
| (3,2727) | 1:76:A:GLU:HB2 | 1:77:A:GLY:H   | 36       | 0.17          |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2  | 8        | 0.17          |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2  | 9        | 0.17          |
| (3,2679) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 1        | 0.17          |
| (3,2679) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 14       | 0.17          |
| (3,2679) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 39       | 0.17          |
| (3,2619) | 1:74:A:ASP:HB3 | 1:74:A:ASP:H   | 17       | 0.17          |
| (3,2602) | 1:36:A:ASP:HB2 | 1:37:A:ASP:H   | 7        | 0.17          |
| (3,2554) | 1:92:A:ARG:HA  | 1:83:A:ALA:H   | 32       | 0.17          |
| (3,2514) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 7        | 0.17          |
| (3,2514) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 17       | 0.17          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 1        | 0.17          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 5        | 0.17          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 6        | 0.17          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 19       | 0.17          |
| (3,2463) | 1:4:A:PRO:HD3  | 1:3:A:ASP:HA   | 28       | 0.17          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,2463) | 1:4:A:PRO:HD3  | 1:3:A:ASP:HA   | 38       | 0.17          |
| (3,2434) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 2        | 0.17          |
| (3,2434) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 18       | 0.17          |
| (3,2412) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 2        | 0.17          |
| (3,2412) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 3        | 0.17          |
| (3,2412) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 5        | 0.17          |
| (3,2412) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 18       | 0.17          |
| (3,2412) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 24       | 0.17          |
| (3,2412) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 30       | 0.17          |
| (3,2412) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 38       | 0.17          |
| (3,2406) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 34       | 0.17          |
| (3,2406) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 34       | 0.17          |
| (3,2406) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 34       | 0.17          |
| (3,2406) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 36       | 0.17          |
| (3,2406) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 36       | 0.17          |
| (3,2406) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 36       | 0.17          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 8        | 0.17          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 8        | 0.17          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 8        | 0.17          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 11       | 0.17          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 11       | 0.17          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 11       | 0.17          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 18       | 0.17          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 18       | 0.17          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 18       | 0.17          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 22       | 0.17          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 22       | 0.17          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 22       | 0.17          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 26       | 0.17          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 26       | 0.17          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 26       | 0.17          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 31       | 0.17          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 31       | 0.17          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 31       | 0.17          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 32       | 0.17          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 32       | 0.17          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 32       | 0.17          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 36       | 0.17          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 36       | 0.17          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 36       | 0.17          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1 | 32       | 0.17          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2 | 32       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2240) | 1:18:A:ASN:HB2  | 1:18:A:ASN:H    | 37       | 0.17          |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 13       | 0.17          |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 31       | 0.17          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 3        | 0.17          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 3        | 0.17          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 3        | 0.17          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 10       | 0.17          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 10       | 0.17          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 10       | 0.17          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 13       | 0.17          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 13       | 0.17          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 13       | 0.17          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 24       | 0.17          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 24       | 0.17          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 24       | 0.17          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 29       | 0.17          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 29       | 0.17          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 29       | 0.17          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 33       | 0.17          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 33       | 0.17          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 33       | 0.17          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 36       | 0.17          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 36       | 0.17          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 36       | 0.17          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 40       | 0.17          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 40       | 0.17          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 40       | 0.17          |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD11 | 17       | 0.17          |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD12 | 17       | 0.17          |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD13 | 17       | 0.17          |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD11 | 17       | 0.17          |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD12 | 17       | 0.17          |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD13 | 17       | 0.17          |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD11 | 17       | 0.17          |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD12 | 17       | 0.17          |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD13 | 17       | 0.17          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1  | 1        | 0.17          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2  | 1        | 0.17          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1  | 1        | 0.17          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2  | 1        | 0.17          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1  | 1        | 0.17          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2  | 1        | 0.17          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 1        | 0.17          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 1        | 0.17          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 1        | 0.17          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 4        | 0.17          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 4        | 0.17          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 4        | 0.17          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 18       | 0.17          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 18       | 0.17          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 18       | 0.17          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 21       | 0.17          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 21       | 0.17          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 21       | 0.17          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 22       | 0.17          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 22       | 0.17          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 22       | 0.17          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 31       | 0.17          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 31       | 0.17          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 31       | 0.17          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 35       | 0.17          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 35       | 0.17          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 35       | 0.17          |
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 13       | 0.17          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 13       | 0.17          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 13       | 0.17          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 17       | 0.17          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 17       | 0.17          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 17       | 0.17          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 17       | 0.17          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 17       | 0.17          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 17       | 0.17          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 22       | 0.17          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 22       | 0.17          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 22       | 0.17          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 22       | 0.17          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 22       | 0.17          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 22       | 0.17          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 25       | 0.17          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 25       | 0.17          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 25       | 0.17          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 25       | 0.17          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 25       | 0.17          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 25       | 0.17          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 34       | 0.17          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 34       | 0.17          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 34       | 0.17          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 34       | 0.17          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 34       | 0.17          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 34       | 0.17          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 17       | 0.17          |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2 | 17       | 0.17          |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2 | 17       | 0.17          |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2 | 17       | 0.17          |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2 | 30       | 0.17          |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2 | 30       | 0.17          |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2 | 30       | 0.17          |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2 | 36       | 0.17          |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2 | 36       | 0.17          |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2 | 36       | 0.17          |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2 | 37       | 0.17          |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2 | 37       | 0.17          |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2 | 37       | 0.17          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA  | 1        | 0.17          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA  | 9        | 0.17          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA  | 12       | 0.17          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA  | 16       | 0.17          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA  | 40       | 0.17          |
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 36       | 0.17          |
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 36       | 0.17          |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 36       | 0.17          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H   | 29       | 0.17          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H   | 29       | 0.17          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H   | 29       | 0.17          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 1        | 0.17          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 1        | 0.17          |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 1        | 0.17          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 7        | 0.17          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 7        | 0.17          |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 7        | 0.17          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 13       | 0.17          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 13       | 0.17          |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 13       | 0.17          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 21       | 0.17          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 21       | 0.17          |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 21       | 0.17          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,1856) | 1:27:A:ALA:HB1 | 1:28:A:THR:H   | 23       | 0.17          |
| (3,1856) | 1:27:A:ALA:HB2 | 1:28:A:THR:H   | 23       | 0.17          |
| (3,1856) | 1:27:A:ALA:HB3 | 1:28:A:THR:H   | 23       | 0.17          |
| (3,1856) | 1:27:A:ALA:HB1 | 1:28:A:THR:H   | 24       | 0.17          |
| (3,1856) | 1:27:A:ALA:HB2 | 1:28:A:THR:H   | 24       | 0.17          |
| (3,1856) | 1:27:A:ALA:HB3 | 1:28:A:THR:H   | 24       | 0.17          |
| (3,1856) | 1:27:A:ALA:HB1 | 1:28:A:THR:H   | 36       | 0.17          |
| (3,1856) | 1:27:A:ALA:HB2 | 1:28:A:THR:H   | 36       | 0.17          |
| (3,1856) | 1:27:A:ALA:HB3 | 1:28:A:THR:H   | 36       | 0.17          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3 | 1        | 0.17          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 1        | 0.17          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 2        | 0.17          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 4        | 0.17          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 9        | 0.17          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 10       | 0.17          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 11       | 0.17          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 12       | 0.17          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 13       | 0.17          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 18       | 0.17          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 20       | 0.17          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 21       | 0.17          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 22       | 0.17          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 23       | 0.17          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 25       | 0.17          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 27       | 0.17          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 28       | 0.17          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 29       | 0.17          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 30       | 0.17          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 31       | 0.17          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 32       | 0.17          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 33       | 0.17          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 34       | 0.17          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 36       | 0.17          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 38       | 0.17          |
| (3,1811) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 39       | 0.17          |
| (3,1781) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 21       | 0.17          |
| (3,1781) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 30       | 0.17          |
| (3,1781) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 31       | 0.17          |
| (3,1781) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 33       | 0.17          |
| (3,1781) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 36       | 0.17          |
| (3,1781) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 37       | 0.17          |
| (3,1781) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 40       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1747) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 3        | 0.17          |
| (3,1747) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 4        | 0.17          |
| (3,1747) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 6        | 0.17          |
| (3,1747) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 7        | 0.17          |
| (3,1747) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 12       | 0.17          |
| (3,1747) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 14       | 0.17          |
| (3,1747) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 19       | 0.17          |
| (3,1747) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 23       | 0.17          |
| (3,1747) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 25       | 0.17          |
| (3,1747) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 26       | 0.17          |
| (3,1747) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 28       | 0.17          |
| (3,1747) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 29       | 0.17          |
| (3,1747) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 31       | 0.17          |
| (3,1747) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 32       | 0.17          |
| (3,1747) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 33       | 0.17          |
| (3,1747) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 34       | 0.17          |
| (3,1747) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 35       | 0.17          |
| (3,1747) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 36       | 0.17          |
| (3,1747) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 40       | 0.17          |
| (3,1731) | 1:48:A:GLU:HB2  | 1:48:A:GLU:H    | 20       | 0.17          |
| (3,1721) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG11 | 7        | 0.17          |
| (3,1721) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG12 | 7        | 0.17          |
| (3,1721) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG13 | 7        | 0.17          |
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG11 | 7        | 0.17          |
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG12 | 7        | 0.17          |
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 7        | 0.17          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 7        | 0.17          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 7        | 0.17          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 7        | 0.17          |
| (3,1721) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG11 | 31       | 0.17          |
| (3,1721) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG12 | 31       | 0.17          |
| (3,1721) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG13 | 31       | 0.17          |
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG11 | 31       | 0.17          |
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG12 | 31       | 0.17          |
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 31       | 0.17          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 31       | 0.17          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 31       | 0.17          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 31       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 1        | 0.17          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 1        | 0.17          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 1        | 0.17          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 1        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 1        | 0.17          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 1        | 0.17          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 1        | 0.17          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 1        | 0.17          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 1        | 0.17          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 19       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 19       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 19       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 19       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 19       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 19       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 19       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 19       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 19       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 20       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 20       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 20       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 20       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 20       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 20       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 20       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 20       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 20       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 21       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 21       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 21       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 21       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 21       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 21       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 21       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 21       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 21       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 27       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 27       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 27       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 27       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 27       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 27       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 27       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 27       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 27       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 33       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 33       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 33       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 33       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 33       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 33       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 33       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 33       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 33       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 36       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 36       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 36       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 36       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 36       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 36       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 36       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 36       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 36       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 38       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 38       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 38       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 38       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 38       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 38       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 38       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 38       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 38       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 40       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 40       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 40       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 40       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 40       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 40       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 40       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 40       | 0.17          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 40       | 0.17          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 23       | 0.17          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 23       | 0.17          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 23       | 0.17          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 5        | 0.17          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 5        | 0.17          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 5        | 0.17          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 5        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 5        | 0.17          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 5        | 0.17          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 5        | 0.17          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 5        | 0.17          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 5        | 0.17          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 6        | 0.17          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 6        | 0.17          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 6        | 0.17          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 6        | 0.17          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 6        | 0.17          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 6        | 0.17          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 6        | 0.17          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 6        | 0.17          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 6        | 0.17          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 9        | 0.17          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 9        | 0.17          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 9        | 0.17          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 9        | 0.17          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 9        | 0.17          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 9        | 0.17          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 9        | 0.17          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 9        | 0.17          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 9        | 0.17          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 16       | 0.17          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 16       | 0.17          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 16       | 0.17          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 16       | 0.17          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 16       | 0.17          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 16       | 0.17          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 16       | 0.17          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 16       | 0.17          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 16       | 0.17          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 39       | 0.17          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 39       | 0.17          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 39       | 0.17          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 39       | 0.17          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 39       | 0.17          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 39       | 0.17          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 39       | 0.17          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 39       | 0.17          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 39       | 0.17          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 40       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 40       | 0.17          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 40       | 0.17          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 40       | 0.17          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 40       | 0.17          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 40       | 0.17          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 40       | 0.17          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 40       | 0.17          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 40       | 0.17          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 28       | 0.17          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 28       | 0.17          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 28       | 0.17          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 35       | 0.17          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 35       | 0.17          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 35       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 8        | 0.17          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 8        | 0.17          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 8        | 0.17          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 11       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 11       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 11       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 13       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 13       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 13       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 14       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 14       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 14       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 17       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 17       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 17       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 18       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 18       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 18       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 19       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 19       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 19       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 20       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 20       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 20       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 21       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 21       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 21       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 22       | 0.17          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 22       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 22       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 23       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 23       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 23       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 24       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 24       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 24       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 25       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 25       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 25       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 27       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 27       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 27       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 30       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 30       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 30       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 34       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 34       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 34       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 39       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 39       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 39       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 40       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 40       | 0.17          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 40       | 0.17          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 20       | 0.17          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 20       | 0.17          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 20       | 0.17          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 20       | 0.17          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 20       | 0.17          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 20       | 0.17          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 28       | 0.17          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 28       | 0.17          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 28       | 0.17          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 28       | 0.17          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 28       | 0.17          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 28       | 0.17          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 31       | 0.17          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 31       | 0.17          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 31       | 0.17          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 31       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 31       | 0.17          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 31       | 0.17          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 37       | 0.17          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 37       | 0.17          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 37       | 0.17          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 37       | 0.17          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 37       | 0.17          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 37       | 0.17          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 20       | 0.17          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 20       | 0.17          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 20       | 0.17          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 23       | 0.17          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 23       | 0.17          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 23       | 0.17          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 27       | 0.17          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 27       | 0.17          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 27       | 0.17          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 37       | 0.17          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 37       | 0.17          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 37       | 0.17          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 17       | 0.17          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 17       | 0.17          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 17       | 0.17          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 21       | 0.17          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 21       | 0.17          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 21       | 0.17          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 23       | 0.17          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 23       | 0.17          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 23       | 0.17          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 24       | 0.17          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 24       | 0.17          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 24       | 0.17          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 25       | 0.17          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 25       | 0.17          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 25       | 0.17          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 28       | 0.17          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 28       | 0.17          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 28       | 0.17          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 32       | 0.17          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 32       | 0.17          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 32       | 0.17          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 38       | 0.17          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA  | 38       | 0.17          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA  | 38       | 0.17          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA  | 39       | 0.17          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA  | 39       | 0.17          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA  | 39       | 0.17          |
| (3,1547) | 1:2:A:ILE:HG12  | 1:2:A:ILE:HA   | 36       | 0.17          |
| (3,1547) | 1:2:A:ILE:HG12  | 1:2:A:ILE:HA   | 37       | 0.17          |
| (3,1534) | 1:2:A:ILE:HG21  | 1:2:A:ILE:HA   | 8        | 0.17          |
| (3,1534) | 1:2:A:ILE:HG22  | 1:2:A:ILE:HA   | 8        | 0.17          |
| (3,1534) | 1:2:A:ILE:HG23  | 1:2:A:ILE:HA   | 8        | 0.17          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 1        | 0.17          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 1        | 0.17          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 1        | 0.17          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 14       | 0.17          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 14       | 0.17          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 14       | 0.17          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 22       | 0.17          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 22       | 0.17          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 22       | 0.17          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 38       | 0.17          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 38       | 0.17          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 38       | 0.17          |
| (3,1517) | 1:66:A:MET:HE1  | 1:29:A:PHE:H   | 17       | 0.17          |
| (3,1517) | 1:66:A:MET:HE2  | 1:29:A:PHE:H   | 17       | 0.17          |
| (3,1517) | 1:66:A:MET:HE3  | 1:29:A:PHE:H   | 17       | 0.17          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1 | 9        | 0.17          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2 | 9        | 0.17          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1 | 9        | 0.17          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2 | 9        | 0.17          |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1 | 9        | 0.17          |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2 | 9        | 0.17          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1 | 13       | 0.17          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2 | 13       | 0.17          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1 | 13       | 0.17          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2 | 13       | 0.17          |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1 | 13       | 0.17          |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2 | 13       | 0.17          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1 | 16       | 0.17          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2 | 16       | 0.17          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1 | 16       | 0.17          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2 | 16       | 0.17          |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1 | 16       | 0.17          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2 | 16       | 0.17          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1 | 17       | 0.17          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2 | 17       | 0.17          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1 | 17       | 0.17          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2 | 17       | 0.17          |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1 | 17       | 0.17          |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2 | 17       | 0.17          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1 | 32       | 0.17          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2 | 32       | 0.17          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1 | 32       | 0.17          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2 | 32       | 0.17          |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1 | 32       | 0.17          |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2 | 32       | 0.17          |
| (3,1512) | 1:66:A:MET:HE1  | 1:42:A:TRP:HZ3 | 1        | 0.17          |
| (3,1512) | 1:66:A:MET:HE2  | 1:42:A:TRP:HZ3 | 1        | 0.17          |
| (3,1512) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3 | 1        | 0.17          |
| (3,1512) | 1:66:A:MET:HE1  | 1:42:A:TRP:HZ3 | 5        | 0.17          |
| (3,1512) | 1:66:A:MET:HE2  | 1:42:A:TRP:HZ3 | 5        | 0.17          |
| (3,1512) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3 | 5        | 0.17          |
| (3,1512) | 1:66:A:MET:HE1  | 1:42:A:TRP:HZ3 | 30       | 0.17          |
| (3,1512) | 1:66:A:MET:HE2  | 1:42:A:TRP:HZ3 | 30       | 0.17          |
| (3,1512) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3 | 30       | 0.17          |
| (3,1512) | 1:66:A:MET:HE1  | 1:42:A:TRP:HZ3 | 34       | 0.17          |
| (3,1512) | 1:66:A:MET:HE2  | 1:42:A:TRP:HZ3 | 34       | 0.17          |
| (3,1512) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3 | 34       | 0.17          |
| (3,1504) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2 | 6        | 0.17          |
| (3,1504) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2 | 6        | 0.17          |
| (3,1504) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2 | 6        | 0.17          |
| (3,1504) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2 | 19       | 0.17          |
| (3,1504) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2 | 19       | 0.17          |
| (3,1504) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2 | 19       | 0.17          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 15       | 0.17          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 15       | 0.17          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 15       | 0.17          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 17       | 0.17          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 17       | 0.17          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 17       | 0.17          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 25       | 0.17          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 25       | 0.17          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 25       | 0.17          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 26       | 0.17          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 26       | 0.17          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 26       | 0.17          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 30       | 0.17          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 30       | 0.17          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 30       | 0.17          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 34       | 0.17          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 34       | 0.17          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 34       | 0.17          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 35       | 0.17          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 35       | 0.17          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 35       | 0.17          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 36       | 0.17          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 36       | 0.17          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 36       | 0.17          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 39       | 0.17          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 39       | 0.17          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 39       | 0.17          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 9        | 0.17          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 9        | 0.17          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 9        | 0.17          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 14       | 0.17          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 14       | 0.17          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 14       | 0.17          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 21       | 0.17          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 21       | 0.17          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 21       | 0.17          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 34       | 0.17          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 34       | 0.17          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 34       | 0.17          |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 4        | 0.17          |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 4        | 0.17          |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 4        | 0.17          |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 11       | 0.17          |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 11       | 0.17          |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 11       | 0.17          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 16       | 0.17          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 16       | 0.17          |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 16       | 0.17          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 23       | 0.17          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 23       | 0.17          |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 23       | 0.17          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 31       | 0.17          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 31       | 0.17          |

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| Key      | Atom-1          | Atom-2       | Model ID | Violation (Å) |
|----------|-----------------|--------------|----------|---------------|
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H | 31       | 0.17          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H | 35       | 0.17          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H | 35       | 0.17          |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H | 35       | 0.17          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H | 39       | 0.17          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H | 39       | 0.17          |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H | 39       | 0.17          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H | 40       | 0.17          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H | 40       | 0.17          |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H | 40       | 0.17          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 1        | 0.17          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 1        | 0.17          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 1        | 0.17          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 2        | 0.17          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 2        | 0.17          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 2        | 0.17          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 7        | 0.17          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 7        | 0.17          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 7        | 0.17          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 10       | 0.17          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 10       | 0.17          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 10       | 0.17          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 16       | 0.17          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 16       | 0.17          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 16       | 0.17          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 20       | 0.17          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 20       | 0.17          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 20       | 0.17          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 1        | 0.17          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 1        | 0.17          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 1        | 0.17          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 5        | 0.17          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 5        | 0.17          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 5        | 0.17          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 8        | 0.17          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 8        | 0.17          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 8        | 0.17          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 9        | 0.17          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 9        | 0.17          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 9        | 0.17          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 10       | 0.17          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 10       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H    | 10       | 0.17          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H    | 13       | 0.17          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H    | 13       | 0.17          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H    | 13       | 0.17          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H    | 15       | 0.17          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H    | 15       | 0.17          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H    | 15       | 0.17          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H    | 17       | 0.17          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H    | 17       | 0.17          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H    | 17       | 0.17          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H    | 23       | 0.17          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H    | 23       | 0.17          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H    | 23       | 0.17          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H    | 28       | 0.17          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H    | 28       | 0.17          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H    | 28       | 0.17          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H    | 32       | 0.17          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H    | 32       | 0.17          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H    | 32       | 0.17          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H    | 34       | 0.17          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H    | 34       | 0.17          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H    | 34       | 0.17          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H    | 39       | 0.17          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H    | 39       | 0.17          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H    | 39       | 0.17          |
| (3,1405) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H    | 2        | 0.17          |
| (3,1405) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H    | 2        | 0.17          |
| (3,1405) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H    | 2        | 0.17          |
| (3,1405) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H    | 17       | 0.17          |
| (3,1405) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H    | 17       | 0.17          |
| (3,1405) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H    | 17       | 0.17          |
| (3,1405) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H    | 22       | 0.17          |
| (3,1405) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H    | 22       | 0.17          |
| (3,1405) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H    | 22       | 0.17          |
| (3,1405) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H    | 26       | 0.17          |
| (3,1405) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H    | 26       | 0.17          |
| (3,1405) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H    | 26       | 0.17          |
| (3,1405) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H    | 29       | 0.17          |
| (3,1405) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H    | 29       | 0.17          |
| (3,1405) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H    | 29       | 0.17          |
| (3,1404) | 1:95:A:ALA:HB1  | 1:16:A:ILE:HG12 | 20       | 0.17          |
| (3,1404) | 1:95:A:ALA:HB2  | 1:16:A:ILE:HG12 | 20       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1404) | 1:95:A:ALA:HB3  | 1:16:A:ILE:HG12 | 20       | 0.17          |
| (3,1404) | 1:95:A:ALA:HB1  | 1:16:A:ILE:HG12 | 21       | 0.17          |
| (3,1404) | 1:95:A:ALA:HB2  | 1:16:A:ILE:HG12 | 21       | 0.17          |
| (3,1404) | 1:95:A:ALA:HB3  | 1:16:A:ILE:HG12 | 21       | 0.17          |
| (3,1404) | 1:95:A:ALA:HB1  | 1:16:A:ILE:HG12 | 35       | 0.17          |
| (3,1404) | 1:95:A:ALA:HB2  | 1:16:A:ILE:HG12 | 35       | 0.17          |
| (3,1404) | 1:95:A:ALA:HB3  | 1:16:A:ILE:HG12 | 35       | 0.17          |
| (3,1391) | 1:91:A:ALA:HB1  | 1:12:A:PHE:HZ   | 27       | 0.17          |
| (3,1391) | 1:91:A:ALA:HB2  | 1:12:A:PHE:HZ   | 27       | 0.17          |
| (3,1391) | 1:91:A:ALA:HB3  | 1:12:A:PHE:HZ   | 27       | 0.17          |
| (3,1388) | 1:91:A:ALA:HB1  | 1:83:A:ALA:HB1  | 3        | 0.17          |
| (3,1388) | 1:91:A:ALA:HB1  | 1:83:A:ALA:HB2  | 3        | 0.17          |
| (3,1388) | 1:91:A:ALA:HB1  | 1:83:A:ALA:HB3  | 3        | 0.17          |
| (3,1388) | 1:91:A:ALA:HB2  | 1:83:A:ALA:HB1  | 3        | 0.17          |
| (3,1388) | 1:91:A:ALA:HB2  | 1:83:A:ALA:HB2  | 3        | 0.17          |
| (3,1388) | 1:91:A:ALA:HB2  | 1:83:A:ALA:HB3  | 3        | 0.17          |
| (3,1388) | 1:91:A:ALA:HB3  | 1:83:A:ALA:HB1  | 3        | 0.17          |
| (3,1388) | 1:91:A:ALA:HB3  | 1:83:A:ALA:HB2  | 3        | 0.17          |
| (3,1388) | 1:91:A:ALA:HB3  | 1:83:A:ALA:HB3  | 3        | 0.17          |
| (3,1383) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB1  | 3        | 0.17          |
| (3,1383) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB2  | 3        | 0.17          |
| (3,1383) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB3  | 3        | 0.17          |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB1  | 3        | 0.17          |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB2  | 3        | 0.17          |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB3  | 3        | 0.17          |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB1  | 3        | 0.17          |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB2  | 3        | 0.17          |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB3  | 3        | 0.17          |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 13       | 0.17          |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 22       | 0.17          |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 26       | 0.17          |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 31       | 0.17          |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 38       | 0.17          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 2        | 0.17          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 2        | 0.17          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 2        | 0.17          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 4        | 0.17          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 4        | 0.17          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 4        | 0.17          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 8        | 0.17          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 8        | 0.17          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 8        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 10       | 0.17          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 10       | 0.17          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 10       | 0.17          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 12       | 0.17          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 12       | 0.17          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 12       | 0.17          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 27       | 0.17          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 27       | 0.17          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 27       | 0.17          |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 2        | 0.17          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 3        | 0.17          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 3        | 0.17          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 3        | 0.17          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 14       | 0.17          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 14       | 0.17          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 14       | 0.17          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 15       | 0.17          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 15       | 0.17          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 15       | 0.17          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 18       | 0.17          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 18       | 0.17          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 18       | 0.17          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 26       | 0.17          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 26       | 0.17          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 26       | 0.17          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 40       | 0.17          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 40       | 0.17          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 40       | 0.17          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 3        | 0.17          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 3        | 0.17          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 3        | 0.17          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 14       | 0.17          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 14       | 0.17          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 14       | 0.17          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 15       | 0.17          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 15       | 0.17          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 15       | 0.17          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 18       | 0.17          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 18       | 0.17          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 18       | 0.17          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 26       | 0.17          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 26       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 26       | 0.17          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 40       | 0.17          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 40       | 0.17          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 40       | 0.17          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 14       | 0.17          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 14       | 0.17          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 14       | 0.17          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 14       | 0.17          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 14       | 0.17          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 14       | 0.17          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 14       | 0.17          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 14       | 0.17          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 14       | 0.17          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 6        | 0.17          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 6        | 0.17          |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 6        | 0.17          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 19       | 0.17          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 19       | 0.17          |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 19       | 0.17          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 20       | 0.17          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 20       | 0.17          |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 20       | 0.17          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 6        | 0.17          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 6        | 0.17          |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 6        | 0.17          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 19       | 0.17          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 19       | 0.17          |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 19       | 0.17          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 20       | 0.17          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 20       | 0.17          |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 20       | 0.17          |
| (3,1261) | 1:67:A:THR:HG21 | 1:26:A:SER:HB2  | 1        | 0.17          |
| (3,1261) | 1:67:A:THR:HG22 | 1:26:A:SER:HB2  | 1        | 0.17          |
| (3,1261) | 1:67:A:THR:HG23 | 1:26:A:SER:HB2  | 1        | 0.17          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 5        | 0.17          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 5        | 0.17          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 5        | 0.17          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 23       | 0.17          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 23       | 0.17          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 23       | 0.17          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 34       | 0.17          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 34       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 34       | 0.17          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 36       | 0.17          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 36       | 0.17          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 36       | 0.17          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 13       | 0.17          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 13       | 0.17          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 13       | 0.17          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 15       | 0.17          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 15       | 0.17          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 15       | 0.17          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 20       | 0.17          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 20       | 0.17          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 20       | 0.17          |
| (3,1243) | 1:13:A:THR:HG21 | 1:34:A:SER:H    | 27       | 0.17          |
| (3,1243) | 1:13:A:THR:HG22 | 1:34:A:SER:H    | 27       | 0.17          |
| (3,1243) | 1:13:A:THR:HG23 | 1:34:A:SER:H    | 27       | 0.17          |
| (3,1240) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3  | 24       | 0.17          |
| (3,1240) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3  | 24       | 0.17          |
| (3,1240) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3  | 24       | 0.17          |
| (3,1230) | 1:101:A:LEU:H   | 1:22:A:SER:HA   | 9        | 0.17          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 3        | 0.17          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 6        | 0.17          |
| (3,1195) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 7        | 0.17          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 18       | 0.17          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 18       | 0.17          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 18       | 0.17          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 19       | 0.17          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 19       | 0.17          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 19       | 0.17          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 20       | 0.17          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 20       | 0.17          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 20       | 0.17          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 23       | 0.17          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 23       | 0.17          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 23       | 0.17          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 25       | 0.17          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 25       | 0.17          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 25       | 0.17          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 27       | 0.17          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 27       | 0.17          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 27       | 0.17          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 30       | 0.17          |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (3,1194) | 1:22:A:SER:H  | 1:21:A:VAL:HG22 | 30       | 0.17          |
| (3,1194) | 1:22:A:SER:H  | 1:21:A:VAL:HG23 | 30       | 0.17          |
| (3,1194) | 1:22:A:SER:H  | 1:21:A:VAL:HG21 | 35       | 0.17          |
| (3,1194) | 1:22:A:SER:H  | 1:21:A:VAL:HG22 | 35       | 0.17          |
| (3,1194) | 1:22:A:SER:H  | 1:21:A:VAL:HG23 | 35       | 0.17          |
| (3,1194) | 1:22:A:SER:H  | 1:21:A:VAL:HG21 | 36       | 0.17          |
| (3,1194) | 1:22:A:SER:H  | 1:21:A:VAL:HG22 | 36       | 0.17          |
| (3,1194) | 1:22:A:SER:H  | 1:21:A:VAL:HG23 | 36       | 0.17          |
| (3,1194) | 1:22:A:SER:H  | 1:21:A:VAL:HG21 | 37       | 0.17          |
| (3,1194) | 1:22:A:SER:H  | 1:21:A:VAL:HG22 | 37       | 0.17          |
| (3,1194) | 1:22:A:SER:H  | 1:21:A:VAL:HG23 | 37       | 0.17          |
| (3,1189) | 1:21:A:VAL:H  | 1:100:A:GLU:HB3 | 11       | 0.17          |
| (3,1189) | 1:21:A:VAL:H  | 1:100:A:GLU:HB3 | 27       | 0.17          |
| (3,1189) | 1:21:A:VAL:H  | 1:100:A:GLU:HB3 | 30       | 0.17          |
| (3,1181) | 1:100:A:GLU:H | 1:21:A:VAL:HG11 | 7        | 0.17          |
| (3,1181) | 1:100:A:GLU:H | 1:21:A:VAL:HG12 | 7        | 0.17          |
| (3,1181) | 1:100:A:GLU:H | 1:21:A:VAL:HG13 | 7        | 0.17          |
| (3,1180) | 1:47:A:THR:H  | 1:44:A:LYS:HB3  | 11       | 0.17          |
| (3,1180) | 1:47:A:THR:H  | 1:44:A:LYS:HB3  | 18       | 0.17          |
| (3,1178) | 1:91:A:ALA:H  | 1:84:A:ARG:HA   | 4        | 0.17          |
| (3,1178) | 1:91:A:ALA:H  | 1:84:A:ARG:HA   | 8        | 0.17          |
| (3,1173) | 1:14:A:LYS:H  | 1:14:A:LYS:HD2  | 7        | 0.17          |
| (3,1167) | 1:75:A:ASP:H  | 1:74:A:ASP:HB2  | 7        | 0.17          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 6        | 0.17          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 6        | 0.17          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 14       | 0.17          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 14       | 0.17          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 16       | 0.17          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 16       | 0.17          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 22       | 0.17          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 22       | 0.17          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 25       | 0.17          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 25       | 0.17          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 28       | 0.17          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 28       | 0.17          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 31       | 0.17          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 31       | 0.17          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 32       | 0.17          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 32       | 0.17          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 33       | 0.17          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 33       | 0.17          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 34       | 0.17          |

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| Key      | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|----------|---------------|----------------|----------|---------------|
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2 | 34       | 0.17          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1 | 37       | 0.17          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2 | 37       | 0.17          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1 | 39       | 0.17          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2 | 39       | 0.17          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1 | 40       | 0.17          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2 | 40       | 0.17          |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 2        | 0.17          |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 16       | 0.17          |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 24       | 0.17          |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 29       | 0.17          |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 33       | 0.17          |
| (3,1126) | 1:78:A:VAL:H  | 1:44:A:LYS:HE2 | 2        | 0.17          |
| (3,1096) | 1:74:A:ASP:H  | 1:73:A:PRO:HA  | 3        | 0.17          |
| (3,1096) | 1:74:A:ASP:H  | 1:73:A:PRO:HA  | 6        | 0.17          |
| (3,1096) | 1:74:A:ASP:H  | 1:73:A:PRO:HA  | 10       | 0.17          |
| (3,1096) | 1:74:A:ASP:H  | 1:73:A:PRO:HA  | 11       | 0.17          |
| (3,1096) | 1:74:A:ASP:H  | 1:73:A:PRO:HA  | 12       | 0.17          |
| (3,1096) | 1:74:A:ASP:H  | 1:73:A:PRO:HA  | 14       | 0.17          |
| (3,1096) | 1:74:A:ASP:H  | 1:73:A:PRO:HA  | 15       | 0.17          |
| (3,1096) | 1:74:A:ASP:H  | 1:73:A:PRO:HA  | 18       | 0.17          |
| (3,1096) | 1:74:A:ASP:H  | 1:73:A:PRO:HA  | 19       | 0.17          |
| (3,1096) | 1:74:A:ASP:H  | 1:73:A:PRO:HA  | 36       | 0.17          |
| (3,1063) | 1:71:A:VAL:H  | 1:25:A:GLN:H   | 17       | 0.17          |
| (3,988)  | 1:12:A:PHE:H  | 1:11:A:GLN:HB2 | 38       | 0.17          |
| (3,968)  | 1:21:A:VAL:H  | 1:99:A:GLY:HA3 | 7        | 0.17          |
| (3,968)  | 1:21:A:VAL:H  | 1:99:A:GLY:HA3 | 15       | 0.17          |
| (3,968)  | 1:21:A:VAL:H  | 1:99:A:GLY:HA3 | 34       | 0.17          |
| (3,942)  | 1:34:A:SER:H  | 1:12:A:PHE:HA  | 15       | 0.17          |
| (3,942)  | 1:34:A:SER:H  | 1:12:A:PHE:HA  | 29       | 0.17          |
| (3,942)  | 1:34:A:SER:H  | 1:12:A:PHE:HA  | 32       | 0.17          |
| (3,942)  | 1:34:A:SER:H  | 1:12:A:PHE:HA  | 38       | 0.17          |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB  | 4        | 0.17          |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB  | 13       | 0.17          |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB  | 24       | 0.17          |
| (3,920)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB2 | 7        | 0.17          |
| (3,889)  | 1:80:A:SER:H  | 1:43:A:TYR:HB3 | 3        | 0.17          |
| (3,889)  | 1:80:A:SER:H  | 1:43:A:TYR:HB3 | 9        | 0.17          |
| (3,889)  | 1:80:A:SER:H  | 1:43:A:TYR:HB3 | 26       | 0.17          |
| (3,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3  | 5        | 0.17          |
| (3,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3  | 6        | 0.17          |
| (3,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3  | 9        | 0.17          |

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| Key     | Atom-1       | Atom-2         | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (3,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3  | 12       | 0.17          |
| (3,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3  | 13       | 0.17          |
| (3,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3  | 18       | 0.17          |
| (3,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2  | 23       | 0.17          |
| (3,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2  | 24       | 0.17          |
| (3,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2  | 25       | 0.17          |
| (3,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2  | 26       | 0.17          |
| (3,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2  | 28       | 0.17          |
| (3,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2  | 29       | 0.17          |
| (3,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2  | 37       | 0.17          |
| (3,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2  | 39       | 0.17          |
| (3,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA   | 7        | 0.17          |
| (3,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA   | 29       | 0.17          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1 | 1        | 0.17          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2 | 1        | 0.17          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3 | 1        | 0.17          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1 | 4        | 0.17          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2 | 4        | 0.17          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3 | 4        | 0.17          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1 | 8        | 0.17          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2 | 8        | 0.17          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3 | 8        | 0.17          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1 | 19       | 0.17          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2 | 19       | 0.17          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3 | 19       | 0.17          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1 | 27       | 0.17          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2 | 27       | 0.17          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3 | 27       | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 3        | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 4        | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 5        | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 6        | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 8        | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 9        | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 10       | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 11       | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 12       | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 13       | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 14       | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 16       | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 17       | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 18       | 0.17          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 19       | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 20       | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 21       | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 22       | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 23       | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 24       | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 25       | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 26       | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 27       | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 28       | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 29       | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 30       | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 31       | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 32       | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 33       | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 34       | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 35       | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 36       | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 37       | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 38       | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 39       | 0.17          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 40       | 0.17          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 19       | 0.17          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 19       | 0.17          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 19       | 0.17          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 27       | 0.17          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 27       | 0.17          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 27       | 0.17          |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 2        | 0.17          |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 4        | 0.17          |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 12       | 0.17          |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 15       | 0.17          |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 16       | 0.17          |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 26       | 0.17          |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 30       | 0.17          |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 31       | 0.17          |
| (3,786) | 1:6:A:THR:H  | 1:6:A:THR:HG21  | 33       | 0.17          |
| (3,786) | 1:6:A:THR:H  | 1:6:A:THR:HG22  | 33       | 0.17          |
| (3,786) | 1:6:A:THR:H  | 1:6:A:THR:HG23  | 33       | 0.17          |
| (3,783) | 1:74:A:ASP:H | 1:74:A:ASP:HB3  | 17       | 0.17          |
| (3,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2  | 5        | 0.17          |
| (3,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2  | 14       | 0.17          |

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| Key     | Atom-1       | Atom-2         | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (3,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 20       | 0.17          |
| (3,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 21       | 0.17          |
| (3,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 26       | 0.17          |
| (3,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 32       | 0.17          |
| (3,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 36       | 0.17          |
| (3,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 40       | 0.17          |
| (3,684) | 1:23:A:GLU:H | 1:23:A:GLU:HB3 | 3        | 0.17          |
| (3,684) | 1:23:A:GLU:H | 1:23:A:GLU:HB3 | 5        | 0.17          |
| (3,684) | 1:23:A:GLU:H | 1:23:A:GLU:HB3 | 20       | 0.17          |
| (3,684) | 1:23:A:GLU:H | 1:23:A:GLU:HB3 | 23       | 0.17          |
| (3,684) | 1:23:A:GLU:H | 1:23:A:GLU:HB3 | 26       | 0.17          |
| (3,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 4        | 0.17          |
| (3,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 6        | 0.17          |
| (3,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 7        | 0.17          |
| (3,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 11       | 0.17          |
| (3,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 15       | 0.17          |
| (3,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 17       | 0.17          |
| (3,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 19       | 0.17          |
| (3,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 20       | 0.17          |
| (3,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 21       | 0.17          |
| (3,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 22       | 0.17          |
| (3,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 23       | 0.17          |
| (3,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 24       | 0.17          |
| (3,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 25       | 0.17          |
| (3,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 28       | 0.17          |
| (3,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 32       | 0.17          |
| (3,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 33       | 0.17          |
| (3,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 34       | 0.17          |
| (3,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 35       | 0.17          |
| (3,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 36       | 0.17          |
| (3,589) | 1:93:A:SER:H | 1:92:A:ARG:HG2 | 17       | 0.17          |
| (3,589) | 1:93:A:SER:H | 1:92:A:ARG:HG2 | 19       | 0.17          |
| (3,589) | 1:93:A:SER:H | 1:92:A:ARG:HG2 | 20       | 0.17          |
| (3,589) | 1:93:A:SER:H | 1:92:A:ARG:HG2 | 31       | 0.17          |
| (3,589) | 1:93:A:SER:H | 1:92:A:ARG:HG2 | 32       | 0.17          |
| (3,589) | 1:93:A:SER:H | 1:92:A:ARG:HG2 | 34       | 0.17          |
| (3,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 3        | 0.17          |
| (3,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 9        | 0.17          |
| (3,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 10       | 0.17          |
| (3,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 13       | 0.17          |
| (3,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 20       | 0.17          |
| (3,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 21       | 0.17          |

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| Key     | Atom-1       | Atom-2         | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (3,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 22       | 0.17          |
| (3,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 23       | 0.17          |
| (3,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 24       | 0.17          |
| (3,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 25       | 0.17          |
| (3,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 26       | 0.17          |
| (3,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 32       | 0.17          |
| (3,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 34       | 0.17          |
| (3,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 35       | 0.17          |
| (3,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 36       | 0.17          |
| (3,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 40       | 0.17          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1 | 4        | 0.17          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2 | 4        | 0.17          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1 | 30       | 0.17          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2 | 30       | 0.17          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1 | 32       | 0.17          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2 | 32       | 0.17          |
| (3,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA  | 37       | 0.17          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 3        | 0.17          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 10       | 0.17          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 17       | 0.17          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 22       | 0.17          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 23       | 0.17          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 25       | 0.17          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 26       | 0.17          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 29       | 0.17          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 30       | 0.17          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 32       | 0.17          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 33       | 0.17          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 35       | 0.17          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 36       | 0.17          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2 | 11       | 0.17          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2 | 20       | 0.17          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2 | 22       | 0.17          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2 | 23       | 0.17          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2 | 27       | 0.17          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H  | 17       | 0.17          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H  | 32       | 0.17          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H  | 37       | 0.17          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H  | 38       | 0.17          |
| (3,513) | 1:67:A:THR:H | 1:66:A:MET:HG3 | 6        | 0.17          |
| (3,513) | 1:67:A:THR:H | 1:66:A:MET:HG3 | 12       | 0.17          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2 | 1        | 0.17          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 5        | 0.17          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 9        | 0.17          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 11       | 0.17          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 13       | 0.17          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 18       | 0.17          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 23       | 0.17          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 25       | 0.17          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 27       | 0.17          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 30       | 0.17          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 32       | 0.17          |
| (3,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 6        | 0.17          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 20       | 0.17          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 27       | 0.17          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 28       | 0.17          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 36       | 0.17          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 4        | 0.17          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 25       | 0.17          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 38       | 0.17          |
| (3,368) | 1:18:A:ASN:H | 1:17:A:GLN:HB3  | 37       | 0.17          |
| (3,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 2        | 0.17          |
| (3,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 30       | 0.17          |
| (3,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 17       | 0.17          |
| (3,274) | 1:66:A:MET:H | 1:66:A:MET:HG3  | 6        | 0.17          |
| (3,274) | 1:66:A:MET:H | 1:66:A:MET:HG3  | 21       | 0.17          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 6        | 0.17          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 6        | 0.17          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 6        | 0.17          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 19       | 0.17          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 19       | 0.17          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 19       | 0.17          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 20       | 0.17          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 20       | 0.17          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 20       | 0.17          |
| (3,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 4        | 0.17          |
| (3,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 7        | 0.17          |
| (3,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 15       | 0.17          |
| (3,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 17       | 0.17          |
| (3,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 18       | 0.17          |
| (3,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 20       | 0.17          |
| (3,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 25       | 0.17          |
| (3,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 26       | 0.17          |
| (3,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 30       | 0.17          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 32       | 0.17          |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 34       | 0.17          |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 37       | 0.17          |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 40       | 0.17          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD1  | 4        | 0.17          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD2  | 4        | 0.17          |
| (3,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 26       | 0.17          |
| (3,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 33       | 0.17          |
| (3,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 36       | 0.17          |
| (3,144) | 1:101:A:LEU:H | 1:100:A:GLU:HB2 | 22       | 0.17          |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 2        | 0.17          |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 16       | 0.17          |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 24       | 0.17          |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 29       | 0.17          |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 33       | 0.17          |
| (3,135) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 8        | 0.17          |
| (3,135) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 37       | 0.17          |
| (3,135) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 38       | 0.17          |
| (3,131) | 1:39:A:ILE:H  | 1:39:A:ILE:HA   | 24       | 0.17          |
| (3,131) | 1:39:A:ILE:H  | 1:39:A:ILE:HA   | 36       | 0.17          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 11       | 0.17          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 14       | 0.17          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 16       | 0.17          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 24       | 0.17          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 29       | 0.17          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 37       | 0.17          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 3        | 0.17          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 4        | 0.17          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 6        | 0.17          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 7        | 0.17          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 12       | 0.17          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 14       | 0.17          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 19       | 0.17          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 23       | 0.17          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 25       | 0.17          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 26       | 0.17          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 28       | 0.17          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 29       | 0.17          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 31       | 0.17          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 32       | 0.17          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 33       | 0.17          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 34       | 0.17          |

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| Key      | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|----------|---------------|----------------|----------|---------------|
| (3,72)   | 1:51:A:GLU:H  | 1:51:A:GLU:HG2 | 35       | 0.17          |
| (3,72)   | 1:51:A:GLU:H  | 1:51:A:GLU:HG2 | 36       | 0.17          |
| (3,72)   | 1:51:A:GLU:H  | 1:51:A:GLU:HG2 | 40       | 0.17          |
| (3,59)   | 1:42:A:TRP:H  | 1:41:A:THR:HB  | 2        | 0.17          |
| (3,59)   | 1:42:A:TRP:H  | 1:41:A:THR:HB  | 5        | 0.17          |
| (3,59)   | 1:42:A:TRP:H  | 1:41:A:THR:HB  | 9        | 0.17          |
| (3,59)   | 1:42:A:TRP:H  | 1:41:A:THR:HB  | 16       | 0.17          |
| (3,59)   | 1:42:A:TRP:H  | 1:41:A:THR:HB  | 17       | 0.17          |
| (3,59)   | 1:42:A:TRP:H  | 1:41:A:THR:HB  | 18       | 0.17          |
| (3,59)   | 1:42:A:TRP:H  | 1:41:A:THR:HB  | 19       | 0.17          |
| (3,59)   | 1:42:A:TRP:H  | 1:41:A:THR:HB  | 25       | 0.17          |
| (3,59)   | 1:42:A:TRP:H  | 1:41:A:THR:HB  | 26       | 0.17          |
| (3,59)   | 1:42:A:TRP:H  | 1:41:A:THR:HB  | 28       | 0.17          |
| (3,59)   | 1:42:A:TRP:H  | 1:41:A:THR:HB  | 29       | 0.17          |
| (3,59)   | 1:42:A:TRP:H  | 1:41:A:THR:HB  | 30       | 0.17          |
| (3,59)   | 1:42:A:TRP:H  | 1:41:A:THR:HB  | 32       | 0.17          |
| (3,59)   | 1:42:A:TRP:H  | 1:41:A:THR:HB  | 34       | 0.17          |
| (3,59)   | 1:42:A:TRP:H  | 1:41:A:THR:HB  | 37       | 0.17          |
| (3,59)   | 1:42:A:TRP:H  | 1:41:A:THR:HB  | 38       | 0.17          |
| (3,59)   | 1:42:A:TRP:H  | 1:41:A:THR:HB  | 39       | 0.17          |
| (3,59)   | 1:42:A:TRP:H  | 1:41:A:THR:HB  | 40       | 0.17          |
| (3,51)   | 1:57:A:PHE:H  | 1:56:A:ASN:HB2 | 1        | 0.17          |
| (3,51)   | 1:57:A:PHE:H  | 1:56:A:ASN:HB2 | 6        | 0.17          |
| (3,51)   | 1:57:A:PHE:H  | 1:56:A:ASN:HB2 | 10       | 0.17          |
| (3,51)   | 1:57:A:PHE:H  | 1:56:A:ASN:HB2 | 12       | 0.17          |
| (3,51)   | 1:57:A:PHE:H  | 1:56:A:ASN:HB2 | 16       | 0.17          |
| (3,51)   | 1:57:A:PHE:H  | 1:56:A:ASN:HB2 | 18       | 0.17          |
| (3,51)   | 1:57:A:PHE:H  | 1:56:A:ASN:HB2 | 22       | 0.17          |
| (3,51)   | 1:57:A:PHE:H  | 1:56:A:ASN:HB2 | 26       | 0.17          |
| (3,51)   | 1:57:A:PHE:H  | 1:56:A:ASN:HB2 | 35       | 0.17          |
| (3,51)   | 1:57:A:PHE:H  | 1:56:A:ASN:HB2 | 40       | 0.17          |
| (3,18)   | 1:89:A:GLY:H  | 1:89:A:GLY:HA3 | 29       | 0.17          |
| (3,18)   | 1:89:A:GLY:H  | 1:89:A:GLY:HA3 | 31       | 0.17          |
| (3,18)   | 1:89:A:GLY:H  | 1:89:A:GLY:HA3 | 33       | 0.17          |
| (3,18)   | 1:89:A:GLY:H  | 1:89:A:GLY:HA3 | 36       | 0.17          |
| (1,3209) | 1:57:A:PHE:HZ | 1:55:A:TYR:HD1 | 4        | 0.17          |
| (1,3209) | 1:57:A:PHE:HZ | 1:55:A:TYR:HD2 | 4        | 0.17          |
| (1,3209) | 1:57:A:PHE:HZ | 1:55:A:TYR:HD1 | 6        | 0.17          |
| (1,3209) | 1:57:A:PHE:HZ | 1:55:A:TYR:HD2 | 6        | 0.17          |
| (1,3209) | 1:57:A:PHE:HZ | 1:55:A:TYR:HD1 | 10       | 0.17          |
| (1,3209) | 1:57:A:PHE:HZ | 1:55:A:TYR:HD2 | 10       | 0.17          |
| (1,3209) | 1:57:A:PHE:HZ | 1:55:A:TYR:HD1 | 15       | 0.17          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 15       | 0.17          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 16       | 0.17          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 16       | 0.17          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 40       | 0.17          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 40       | 0.17          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 1        | 0.17          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 1        | 0.17          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 1        | 0.17          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 1        | 0.17          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 1        | 0.17          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 1        | 0.17          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 19       | 0.17          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 19       | 0.17          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 19       | 0.17          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 19       | 0.17          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 19       | 0.17          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 19       | 0.17          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 20       | 0.17          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 20       | 0.17          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 20       | 0.17          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 20       | 0.17          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 20       | 0.17          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 20       | 0.17          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 30       | 0.17          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 30       | 0.17          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 30       | 0.17          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 30       | 0.17          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 30       | 0.17          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 30       | 0.17          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 33       | 0.17          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 33       | 0.17          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 33       | 0.17          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 33       | 0.17          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 33       | 0.17          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 33       | 0.17          |
| (1,3199) | 1:43:A:TYR:HD1 | 1:80:A:SER:HB2  | 21       | 0.17          |
| (1,3199) | 1:43:A:TYR:HD2 | 1:80:A:SER:HB2  | 21       | 0.17          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 1        | 0.17          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 2        | 0.17          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 21       | 0.17          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 22       | 0.17          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 30       | 0.17          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 33       | 0.17          |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2  | 36       | 0.17          |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2  | 36       | 0.17          |
| (1,3132) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB2  | 5        | 0.17          |
| (1,3132) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB2  | 5        | 0.17          |
| (1,3131) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3  | 17       | 0.17          |
| (1,3131) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3  | 17       | 0.17          |
| (1,3131) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3  | 34       | 0.17          |
| (1,3131) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3  | 34       | 0.17          |
| (1,3127) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HB2  | 22       | 0.17          |
| (1,3127) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HB2  | 22       | 0.17          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 3        | 0.17          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 3        | 0.17          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 9        | 0.17          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 9        | 0.17          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 11       | 0.17          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 11       | 0.17          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 18       | 0.17          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 18       | 0.17          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 26       | 0.17          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 26       | 0.17          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 29       | 0.17          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 29       | 0.17          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 3        | 0.17          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 3        | 0.17          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 9        | 0.17          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 9        | 0.17          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 11       | 0.17          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 11       | 0.17          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 18       | 0.17          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 18       | 0.17          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 26       | 0.17          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 26       | 0.17          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 29       | 0.17          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 29       | 0.17          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 20       | 0.17          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 20       | 0.17          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 20       | 0.17          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 20       | 0.17          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 20       | 0.17          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 20       | 0.17          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 28       | 0.17          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 28       | 0.17          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 28       | 0.17          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 28       | 0.17          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 28       | 0.17          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 28       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 1        | 0.17          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 1        | 0.17          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 1        | 0.17          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 1        | 0.17          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 1        | 0.17          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 1        | 0.17          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 20       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 20       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 20       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 20       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 20       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 20       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 26       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 26       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 26       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 26       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 26       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 26       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 32       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 32       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 32       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 32       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 32       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 32       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 35       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 35       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 35       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 35       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 35       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 35       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 37       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 37       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 37       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 37       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 37       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 37       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 38       | 0.17          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 38       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 38       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 38       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 38       | 0.17          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 38       | 0.17          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 1        | 0.17          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 1        | 0.17          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 1        | 0.17          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 1        | 0.17          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 7        | 0.17          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 7        | 0.17          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 7        | 0.17          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 7        | 0.17          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 11       | 0.17          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 11       | 0.17          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 11       | 0.17          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 11       | 0.17          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 16       | 0.17          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 16       | 0.17          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 16       | 0.17          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 16       | 0.17          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 17       | 0.17          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 17       | 0.17          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 17       | 0.17          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 17       | 0.17          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 12       | 0.17          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 12       | 0.17          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 12       | 0.17          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 12       | 0.17          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 12       | 0.17          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 12       | 0.17          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 21       | 0.17          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 21       | 0.17          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 21       | 0.17          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 21       | 0.17          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 21       | 0.17          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 21       | 0.17          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 1        | 0.17          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 2        | 0.17          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 3        | 0.17          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 4        | 0.17          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 5        | 0.17          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 6        | 0.17          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 11       | 0.17          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 14       | 0.17          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 15       | 0.17          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 17       | 0.17          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 29       | 0.17          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 33       | 0.17          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 34       | 0.17          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 37       | 0.17          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 13       | 0.17          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 13       | 0.17          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 13       | 0.17          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 18       | 0.17          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 18       | 0.17          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 18       | 0.17          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 27       | 0.17          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 27       | 0.17          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 27       | 0.17          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 13       | 0.17          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 13       | 0.17          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 35       | 0.17          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 35       | 0.17          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB2  | 21       | 0.17          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB3  | 21       | 0.17          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB2  | 23       | 0.17          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB3  | 23       | 0.17          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB2  | 24       | 0.17          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB3  | 24       | 0.17          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB2  | 25       | 0.17          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB3  | 25       | 0.17          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB2  | 26       | 0.17          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB3  | 26       | 0.17          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB2  | 28       | 0.17          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB3  | 28       | 0.17          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB2  | 29       | 0.17          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB3  | 29       | 0.17          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB2  | 30       | 0.17          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB3  | 30       | 0.17          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB2  | 32       | 0.17          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB3  | 32       | 0.17          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB2  | 34       | 0.17          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB3  | 34       | 0.17          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB2  | 35       | 0.17          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB3  | 35       | 0.17          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB2  | 36       | 0.17          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB3  | 36       | 0.17          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB2  | 37       | 0.17          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB3  | 37       | 0.17          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB2  | 38       | 0.17          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB3  | 38       | 0.17          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB2  | 39       | 0.17          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB3  | 39       | 0.17          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 14       | 0.17          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 27       | 0.17          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 28       | 0.17          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 31       | 0.17          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 38       | 0.17          |
| (1,3033) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE1  | 15       | 0.17          |
| (1,3033) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE2  | 15       | 0.17          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 1        | 0.17          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 1        | 0.17          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 1        | 0.17          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 8        | 0.17          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 8        | 0.17          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 8        | 0.17          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 38       | 0.17          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 38       | 0.17          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 38       | 0.17          |
| (1,2996) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 6        | 0.17          |
| (1,2996) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 7        | 0.17          |
| (1,2996) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 12       | 0.17          |
| (1,2996) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 20       | 0.17          |
| (1,2996) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 36       | 0.17          |
| (1,2974) | 1:65:A:TYR:HA  | 1:42:A:TRP:HZ2  | 8        | 0.17          |
| (1,2930) | 1:17:A:GLN:HG2 | 1:18:A:ASN:H    | 8        | 0.17          |
| (1,2918) | 1:22:A:SER:HB2 | 1:25:A:GLN:H    | 9        | 0.17          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 1        | 0.17          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 2        | 0.17          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 4        | 0.17          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 9        | 0.17          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 10       | 0.17          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 11       | 0.17          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 12       | 0.17          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3  | 13       | 0.17          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 18       | 0.17          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 20       | 0.17          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 21       | 0.17          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 22       | 0.17          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 23       | 0.17          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 25       | 0.17          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 27       | 0.17          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 28       | 0.17          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 29       | 0.17          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 30       | 0.17          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 31       | 0.17          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 32       | 0.17          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 33       | 0.17          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 34       | 0.17          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 36       | 0.17          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 38       | 0.17          |
| (1,2907) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD3 | 39       | 0.17          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 1        | 0.17          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 2        | 0.17          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 4        | 0.17          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 9        | 0.17          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 10       | 0.17          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 11       | 0.17          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 12       | 0.17          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 13       | 0.17          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 18       | 0.17          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 20       | 0.17          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 21       | 0.17          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 22       | 0.17          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 23       | 0.17          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 25       | 0.17          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 27       | 0.17          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 28       | 0.17          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 29       | 0.17          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 30       | 0.17          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 31       | 0.17          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 32       | 0.17          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 33       | 0.17          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 34       | 0.17          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 36       | 0.17          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 38       | 0.17          |
| (1,2904) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 39       | 0.17          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,2903) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD2 | 18       | 0.17          |
| (1,2859) | 1:92:A:ARG:HB3 | 1:92:A:ARG:H   | 9        | 0.17          |
| (1,2859) | 1:92:A:ARG:HB3 | 1:92:A:ARG:H   | 10       | 0.17          |
| (1,2859) | 1:92:A:ARG:HB3 | 1:92:A:ARG:H   | 12       | 0.17          |
| (1,2859) | 1:92:A:ARG:HB3 | 1:92:A:ARG:H   | 20       | 0.17          |
| (1,2859) | 1:92:A:ARG:HB3 | 1:92:A:ARG:H   | 33       | 0.17          |
| (1,2754) | 1:90:A:GLU:HB3 | 1:91:A:ALA:H   | 6        | 0.17          |
| (1,2754) | 1:90:A:GLU:HB3 | 1:91:A:ALA:H   | 8        | 0.17          |
| (1,2754) | 1:90:A:GLU:HB3 | 1:91:A:ALA:H   | 12       | 0.17          |
| (1,2754) | 1:90:A:GLU:HB3 | 1:91:A:ALA:H   | 20       | 0.17          |
| (1,2754) | 1:90:A:GLU:HB3 | 1:91:A:ALA:H   | 36       | 0.17          |
| (1,2723) | 1:76:A:GLU:HB2 | 1:77:A:GLY:H   | 20       | 0.17          |
| (1,2723) | 1:76:A:GLU:HB2 | 1:77:A:GLY:H   | 27       | 0.17          |
| (1,2723) | 1:76:A:GLU:HB2 | 1:77:A:GLY:H   | 28       | 0.17          |
| (1,2723) | 1:76:A:GLU:HB2 | 1:77:A:GLY:H   | 36       | 0.17          |
| (1,2686) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2  | 8        | 0.17          |
| (1,2686) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2  | 9        | 0.17          |
| (1,2675) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 1        | 0.17          |
| (1,2675) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 14       | 0.17          |
| (1,2675) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 39       | 0.17          |
| (1,2615) | 1:74:A:ASP:HB3 | 1:74:A:ASP:H   | 17       | 0.17          |
| (1,2598) | 1:36:A:ASP:HB2 | 1:37:A:ASP:H   | 7        | 0.17          |
| (1,2550) | 1:92:A:ARG:HA  | 1:83:A:ALA:H   | 32       | 0.17          |
| (1,2511) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 7        | 0.17          |
| (1,2511) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 17       | 0.17          |
| (1,2485) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 1        | 0.17          |
| (1,2485) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 5        | 0.17          |
| (1,2485) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 6        | 0.17          |
| (1,2485) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3  | 19       | 0.17          |
| (1,2460) | 1:4:A:PRO:HD3  | 1:3:A:ASP:HA   | 28       | 0.17          |
| (1,2460) | 1:4:A:PRO:HD3  | 1:3:A:ASP:HA   | 38       | 0.17          |
| (1,2431) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 2        | 0.17          |
| (1,2431) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 18       | 0.17          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 2        | 0.17          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 3        | 0.17          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 5        | 0.17          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 18       | 0.17          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 24       | 0.17          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 30       | 0.17          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 38       | 0.17          |
| (1,2403) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 34       | 0.17          |
| (1,2403) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 34       | 0.17          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2403) | 1:66:A:MET:HE3  | 1:42:A:TRP:H   | 34       | 0.17          |
| (1,2403) | 1:66:A:MET:HE1  | 1:42:A:TRP:H   | 36       | 0.17          |
| (1,2403) | 1:66:A:MET:HE2  | 1:42:A:TRP:H   | 36       | 0.17          |
| (1,2403) | 1:66:A:MET:HE3  | 1:42:A:TRP:H   | 36       | 0.17          |
| (1,2402) | 1:66:A:MET:HE1  | 1:29:A:PHE:HZ  | 8        | 0.17          |
| (1,2402) | 1:66:A:MET:HE2  | 1:29:A:PHE:HZ  | 8        | 0.17          |
| (1,2402) | 1:66:A:MET:HE3  | 1:29:A:PHE:HZ  | 8        | 0.17          |
| (1,2402) | 1:66:A:MET:HE1  | 1:29:A:PHE:HZ  | 11       | 0.17          |
| (1,2402) | 1:66:A:MET:HE2  | 1:29:A:PHE:HZ  | 11       | 0.17          |
| (1,2402) | 1:66:A:MET:HE3  | 1:29:A:PHE:HZ  | 11       | 0.17          |
| (1,2402) | 1:66:A:MET:HE1  | 1:29:A:PHE:HZ  | 18       | 0.17          |
| (1,2402) | 1:66:A:MET:HE2  | 1:29:A:PHE:HZ  | 18       | 0.17          |
| (1,2402) | 1:66:A:MET:HE3  | 1:29:A:PHE:HZ  | 18       | 0.17          |
| (1,2402) | 1:66:A:MET:HE1  | 1:29:A:PHE:HZ  | 22       | 0.17          |
| (1,2402) | 1:66:A:MET:HE2  | 1:29:A:PHE:HZ  | 22       | 0.17          |
| (1,2402) | 1:66:A:MET:HE3  | 1:29:A:PHE:HZ  | 22       | 0.17          |
| (1,2402) | 1:66:A:MET:HE1  | 1:29:A:PHE:HZ  | 26       | 0.17          |
| (1,2402) | 1:66:A:MET:HE2  | 1:29:A:PHE:HZ  | 26       | 0.17          |
| (1,2402) | 1:66:A:MET:HE3  | 1:29:A:PHE:HZ  | 26       | 0.17          |
| (1,2402) | 1:66:A:MET:HE1  | 1:29:A:PHE:HZ  | 31       | 0.17          |
| (1,2402) | 1:66:A:MET:HE2  | 1:29:A:PHE:HZ  | 31       | 0.17          |
| (1,2402) | 1:66:A:MET:HE3  | 1:29:A:PHE:HZ  | 31       | 0.17          |
| (1,2402) | 1:66:A:MET:HE1  | 1:29:A:PHE:HZ  | 32       | 0.17          |
| (1,2402) | 1:66:A:MET:HE2  | 1:29:A:PHE:HZ  | 32       | 0.17          |
| (1,2402) | 1:66:A:MET:HE3  | 1:29:A:PHE:HZ  | 32       | 0.17          |
| (1,2402) | 1:66:A:MET:HE1  | 1:29:A:PHE:HZ  | 36       | 0.17          |
| (1,2402) | 1:66:A:MET:HE2  | 1:29:A:PHE:HZ  | 36       | 0.17          |
| (1,2402) | 1:66:A:MET:HE3  | 1:29:A:PHE:HZ  | 36       | 0.17          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1 | 32       | 0.17          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2 | 32       | 0.17          |
| (1,2237) | 1:18:A:ASN:HB2  | 1:18:A:ASN:H   | 37       | 0.17          |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H   | 13       | 0.17          |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H   | 31       | 0.17          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2 | 3        | 0.17          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2 | 3        | 0.17          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2 | 3        | 0.17          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2 | 10       | 0.17          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2 | 10       | 0.17          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2 | 10       | 0.17          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2 | 13       | 0.17          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2 | 13       | 0.17          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2 | 13       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 24       | 0.17          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 24       | 0.17          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 24       | 0.17          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 29       | 0.17          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 29       | 0.17          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 29       | 0.17          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 33       | 0.17          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 33       | 0.17          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 33       | 0.17          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 36       | 0.17          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 36       | 0.17          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 36       | 0.17          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 40       | 0.17          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 40       | 0.17          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 40       | 0.17          |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD11 | 17       | 0.17          |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD12 | 17       | 0.17          |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD13 | 17       | 0.17          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD11 | 17       | 0.17          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD12 | 17       | 0.17          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD13 | 17       | 0.17          |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD11 | 17       | 0.17          |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD12 | 17       | 0.17          |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD13 | 17       | 0.17          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3  | 10       | 0.17          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3  | 10       | 0.17          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3  | 10       | 0.17          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3  | 14       | 0.17          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3  | 14       | 0.17          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3  | 14       | 0.17          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3  | 19       | 0.17          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3  | 19       | 0.17          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3  | 19       | 0.17          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1  | 1        | 0.17          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2  | 1        | 0.17          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1  | 1        | 0.17          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2  | 1        | 0.17          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1  | 1        | 0.17          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2  | 1        | 0.17          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 1        | 0.17          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 1        | 0.17          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 1        | 0.17          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 4        | 0.17          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 4        | 0.17          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 4        | 0.17          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 18       | 0.17          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 18       | 0.17          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 18       | 0.17          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 21       | 0.17          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 21       | 0.17          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 21       | 0.17          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 22       | 0.17          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 22       | 0.17          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 22       | 0.17          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 31       | 0.17          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 31       | 0.17          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 31       | 0.17          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 35       | 0.17          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 35       | 0.17          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 35       | 0.17          |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 13       | 0.17          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 13       | 0.17          |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 13       | 0.17          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 17       | 0.17          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 17       | 0.17          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 17       | 0.17          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 17       | 0.17          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 17       | 0.17          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 17       | 0.17          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 22       | 0.17          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 22       | 0.17          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 22       | 0.17          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 22       | 0.17          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 22       | 0.17          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 22       | 0.17          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 25       | 0.17          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 25       | 0.17          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 25       | 0.17          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 25       | 0.17          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 25       | 0.17          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 25       | 0.17          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 34       | 0.17          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 34       | 0.17          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 34       | 0.17          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 34       | 0.17          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 34       | 0.17          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 34       | 0.17          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 17       | 0.17          |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2 | 17       | 0.17          |
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2 | 17       | 0.17          |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2 | 17       | 0.17          |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2 | 30       | 0.17          |
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2 | 30       | 0.17          |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2 | 30       | 0.17          |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2 | 36       | 0.17          |
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2 | 36       | 0.17          |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2 | 36       | 0.17          |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2 | 37       | 0.17          |
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2 | 37       | 0.17          |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2 | 37       | 0.17          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA  | 1        | 0.17          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA  | 9        | 0.17          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA  | 12       | 0.17          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA  | 16       | 0.17          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA  | 40       | 0.17          |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 36       | 0.17          |
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 36       | 0.17          |
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 36       | 0.17          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H   | 29       | 0.17          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H   | 29       | 0.17          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H   | 29       | 0.17          |
| (1,1853) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 1        | 0.17          |
| (1,1853) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 1        | 0.17          |
| (1,1853) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 1        | 0.17          |
| (1,1853) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 7        | 0.17          |
| (1,1853) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 7        | 0.17          |
| (1,1853) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 7        | 0.17          |
| (1,1853) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 13       | 0.17          |
| (1,1853) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 13       | 0.17          |
| (1,1853) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 13       | 0.17          |
| (1,1853) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 21       | 0.17          |
| (1,1853) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 21       | 0.17          |
| (1,1853) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 21       | 0.17          |
| (1,1853) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 23       | 0.17          |
| (1,1853) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 23       | 0.17          |
| (1,1853) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 23       | 0.17          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1853) | 1:27:A:ALA:HB1 | 1:28:A:THR:H   | 24       | 0.17          |
| (1,1853) | 1:27:A:ALA:HB2 | 1:28:A:THR:H   | 24       | 0.17          |
| (1,1853) | 1:27:A:ALA:HB3 | 1:28:A:THR:H   | 24       | 0.17          |
| (1,1853) | 1:27:A:ALA:HB1 | 1:28:A:THR:H   | 36       | 0.17          |
| (1,1853) | 1:27:A:ALA:HB2 | 1:28:A:THR:H   | 36       | 0.17          |
| (1,1853) | 1:27:A:ALA:HB3 | 1:28:A:THR:H   | 36       | 0.17          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3 | 1        | 0.17          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 1        | 0.17          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 2        | 0.17          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 4        | 0.17          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 9        | 0.17          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 10       | 0.17          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 11       | 0.17          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 12       | 0.17          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 13       | 0.17          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 18       | 0.17          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 20       | 0.17          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 21       | 0.17          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 22       | 0.17          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 23       | 0.17          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 25       | 0.17          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 27       | 0.17          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 28       | 0.17          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 29       | 0.17          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 30       | 0.17          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 31       | 0.17          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 32       | 0.17          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 33       | 0.17          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 34       | 0.17          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 36       | 0.17          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 38       | 0.17          |
| (1,1808) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HE3 | 39       | 0.17          |
| (1,1778) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 21       | 0.17          |
| (1,1778) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 30       | 0.17          |
| (1,1778) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 31       | 0.17          |
| (1,1778) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 33       | 0.17          |
| (1,1778) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 36       | 0.17          |
| (1,1778) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 37       | 0.17          |
| (1,1778) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 40       | 0.17          |
| (1,1744) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H   | 3        | 0.17          |
| (1,1744) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H   | 4        | 0.17          |
| (1,1744) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H   | 6        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1744) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 7        | 0.17          |
| (1,1744) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 12       | 0.17          |
| (1,1744) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 14       | 0.17          |
| (1,1744) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 19       | 0.17          |
| (1,1744) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 23       | 0.17          |
| (1,1744) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 25       | 0.17          |
| (1,1744) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 26       | 0.17          |
| (1,1744) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 28       | 0.17          |
| (1,1744) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 29       | 0.17          |
| (1,1744) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 31       | 0.17          |
| (1,1744) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 32       | 0.17          |
| (1,1744) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 33       | 0.17          |
| (1,1744) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 34       | 0.17          |
| (1,1744) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 35       | 0.17          |
| (1,1744) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 36       | 0.17          |
| (1,1744) | 1:51:A:GLU:HG2  | 1:51:A:GLU:H    | 40       | 0.17          |
| (1,1728) | 1:48:A:GLU:HB2  | 1:48:A:GLU:H    | 20       | 0.17          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG11 | 7        | 0.17          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG12 | 7        | 0.17          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG13 | 7        | 0.17          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG11 | 7        | 0.17          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG12 | 7        | 0.17          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 7        | 0.17          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 7        | 0.17          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 7        | 0.17          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 7        | 0.17          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG11 | 31       | 0.17          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG12 | 31       | 0.17          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG13 | 31       | 0.17          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG11 | 31       | 0.17          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG12 | 31       | 0.17          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 31       | 0.17          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 31       | 0.17          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 31       | 0.17          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 31       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 1        | 0.17          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 1        | 0.17          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 1        | 0.17          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 1        | 0.17          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 1        | 0.17          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 1        | 0.17          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 1        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 1        | 0.17          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 1        | 0.17          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 19       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 19       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 19       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 19       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 19       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 19       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 19       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 19       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 19       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 20       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 20       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 20       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 20       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 20       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 20       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 20       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 20       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 20       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 21       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 21       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 21       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 21       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 21       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 21       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 21       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 21       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 21       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 27       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 27       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 27       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 27       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 27       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 27       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 27       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 27       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 27       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 33       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 33       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 33       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 33       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 33       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 33       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 33       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 33       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 33       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 36       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 36       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 36       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 36       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 36       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 36       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 36       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 36       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 36       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 38       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 38       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 38       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 38       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 38       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 38       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 38       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 38       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 38       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 40       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 40       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 40       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 40       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 40       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 40       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 40       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 40       | 0.17          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 40       | 0.17          |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 23       | 0.17          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 23       | 0.17          |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 23       | 0.17          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 5        | 0.17          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 5        | 0.17          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 5        | 0.17          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 5        | 0.17          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 5        | 0.17          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 5        | 0.17          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 5        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 5        | 0.17          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 5        | 0.17          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 6        | 0.17          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 6        | 0.17          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 6        | 0.17          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 6        | 0.17          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 6        | 0.17          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 6        | 0.17          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 6        | 0.17          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 6        | 0.17          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 6        | 0.17          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 9        | 0.17          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 9        | 0.17          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 9        | 0.17          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 9        | 0.17          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 9        | 0.17          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 9        | 0.17          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 9        | 0.17          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 9        | 0.17          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 9        | 0.17          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 16       | 0.17          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 16       | 0.17          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 16       | 0.17          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 16       | 0.17          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 16       | 0.17          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 16       | 0.17          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 16       | 0.17          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 16       | 0.17          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 16       | 0.17          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 39       | 0.17          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 39       | 0.17          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 39       | 0.17          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 39       | 0.17          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 39       | 0.17          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 39       | 0.17          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 39       | 0.17          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 39       | 0.17          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 39       | 0.17          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 40       | 0.17          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 40       | 0.17          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 40       | 0.17          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 40       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 40       | 0.17          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 40       | 0.17          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 40       | 0.17          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 40       | 0.17          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 40       | 0.17          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 28       | 0.17          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 28       | 0.17          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 28       | 0.17          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 35       | 0.17          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 35       | 0.17          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 35       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 8        | 0.17          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 8        | 0.17          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 8        | 0.17          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 11       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 11       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 11       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 13       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 13       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 13       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 14       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 14       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 14       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 17       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 17       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 17       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 18       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 18       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 18       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 19       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 19       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 19       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 20       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 20       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 20       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 21       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 21       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 21       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 22       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 22       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 22       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 23       | 0.17          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 23       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 23       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 24       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 24       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 24       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 25       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 25       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 25       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 27       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 27       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 27       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 30       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 30       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 30       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 34       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 34       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 34       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 39       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 39       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 39       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA  | 40       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA  | 40       | 0.17          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA  | 40       | 0.17          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 20       | 0.17          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 20       | 0.17          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 20       | 0.17          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 20       | 0.17          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 20       | 0.17          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 20       | 0.17          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 28       | 0.17          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 28       | 0.17          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 28       | 0.17          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 28       | 0.17          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 28       | 0.17          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 28       | 0.17          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 31       | 0.17          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 31       | 0.17          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 31       | 0.17          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 31       | 0.17          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 31       | 0.17          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 31       | 0.17          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 37       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 37       | 0.17          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 37       | 0.17          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 37       | 0.17          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 37       | 0.17          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 37       | 0.17          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 20       | 0.17          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 20       | 0.17          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 20       | 0.17          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 23       | 0.17          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 23       | 0.17          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 23       | 0.17          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 27       | 0.17          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 27       | 0.17          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 27       | 0.17          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 37       | 0.17          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 37       | 0.17          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 37       | 0.17          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 17       | 0.17          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 17       | 0.17          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 17       | 0.17          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 21       | 0.17          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 21       | 0.17          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 21       | 0.17          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 23       | 0.17          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 23       | 0.17          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 23       | 0.17          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 24       | 0.17          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 24       | 0.17          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 24       | 0.17          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 25       | 0.17          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 25       | 0.17          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 25       | 0.17          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 28       | 0.17          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 28       | 0.17          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 28       | 0.17          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 32       | 0.17          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 32       | 0.17          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 32       | 0.17          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 38       | 0.17          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 38       | 0.17          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 38       | 0.17          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 39       | 0.17          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA  | 39       | 0.17          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA  | 39       | 0.17          |
| (1,1543) | 1:2:A:ILE:HG12  | 1:2:A:ILE:HA   | 36       | 0.17          |
| (1,1543) | 1:2:A:ILE:HG12  | 1:2:A:ILE:HA   | 37       | 0.17          |
| (1,1530) | 1:2:A:ILE:HG21  | 1:2:A:ILE:HA   | 8        | 0.17          |
| (1,1530) | 1:2:A:ILE:HG22  | 1:2:A:ILE:HA   | 8        | 0.17          |
| (1,1530) | 1:2:A:ILE:HG23  | 1:2:A:ILE:HA   | 8        | 0.17          |
| (1,1514) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 1        | 0.17          |
| (1,1514) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 1        | 0.17          |
| (1,1514) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 1        | 0.17          |
| (1,1514) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 14       | 0.17          |
| (1,1514) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 14       | 0.17          |
| (1,1514) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 14       | 0.17          |
| (1,1514) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 22       | 0.17          |
| (1,1514) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 22       | 0.17          |
| (1,1514) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 22       | 0.17          |
| (1,1514) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 38       | 0.17          |
| (1,1514) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 38       | 0.17          |
| (1,1514) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 38       | 0.17          |
| (1,1513) | 1:66:A:MET:HE1  | 1:29:A:PHE:H   | 17       | 0.17          |
| (1,1513) | 1:66:A:MET:HE2  | 1:29:A:PHE:H   | 17       | 0.17          |
| (1,1513) | 1:66:A:MET:HE3  | 1:29:A:PHE:H   | 17       | 0.17          |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1 | 9        | 0.17          |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2 | 9        | 0.17          |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1 | 9        | 0.17          |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2 | 9        | 0.17          |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1 | 9        | 0.17          |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2 | 9        | 0.17          |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1 | 13       | 0.17          |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2 | 13       | 0.17          |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1 | 13       | 0.17          |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2 | 13       | 0.17          |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1 | 13       | 0.17          |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2 | 13       | 0.17          |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1 | 16       | 0.17          |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2 | 16       | 0.17          |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1 | 16       | 0.17          |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2 | 16       | 0.17          |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1 | 16       | 0.17          |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2 | 16       | 0.17          |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1 | 17       | 0.17          |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2 | 17       | 0.17          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1 | 17       | 0.17          |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2 | 17       | 0.17          |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1 | 17       | 0.17          |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2 | 17       | 0.17          |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1 | 32       | 0.17          |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2 | 32       | 0.17          |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1 | 32       | 0.17          |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2 | 32       | 0.17          |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1 | 32       | 0.17          |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2 | 32       | 0.17          |
| (1,1508) | 1:66:A:MET:HE1  | 1:42:A:TRP:HZ3 | 1        | 0.17          |
| (1,1508) | 1:66:A:MET:HE2  | 1:42:A:TRP:HZ3 | 1        | 0.17          |
| (1,1508) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3 | 1        | 0.17          |
| (1,1508) | 1:66:A:MET:HE1  | 1:42:A:TRP:HZ3 | 5        | 0.17          |
| (1,1508) | 1:66:A:MET:HE2  | 1:42:A:TRP:HZ3 | 5        | 0.17          |
| (1,1508) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3 | 5        | 0.17          |
| (1,1508) | 1:66:A:MET:HE1  | 1:42:A:TRP:HZ3 | 30       | 0.17          |
| (1,1508) | 1:66:A:MET:HE2  | 1:42:A:TRP:HZ3 | 30       | 0.17          |
| (1,1508) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3 | 30       | 0.17          |
| (1,1508) | 1:66:A:MET:HE1  | 1:42:A:TRP:HZ3 | 34       | 0.17          |
| (1,1508) | 1:66:A:MET:HE2  | 1:42:A:TRP:HZ3 | 34       | 0.17          |
| (1,1508) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3 | 34       | 0.17          |
| (1,1500) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2 | 6        | 0.17          |
| (1,1500) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2 | 6        | 0.17          |
| (1,1500) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2 | 6        | 0.17          |
| (1,1500) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2 | 19       | 0.17          |
| (1,1500) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2 | 19       | 0.17          |
| (1,1500) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2 | 19       | 0.17          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 15       | 0.17          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 15       | 0.17          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 15       | 0.17          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 17       | 0.17          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 17       | 0.17          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 17       | 0.17          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 25       | 0.17          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 25       | 0.17          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 25       | 0.17          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 26       | 0.17          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 26       | 0.17          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 26       | 0.17          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 30       | 0.17          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 30       | 0.17          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 30       | 0.17          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 34       | 0.17          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 34       | 0.17          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 34       | 0.17          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 35       | 0.17          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 35       | 0.17          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 35       | 0.17          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 36       | 0.17          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 36       | 0.17          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 36       | 0.17          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 39       | 0.17          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 39       | 0.17          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 39       | 0.17          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 9        | 0.17          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 9        | 0.17          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 9        | 0.17          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 14       | 0.17          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 14       | 0.17          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 14       | 0.17          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 21       | 0.17          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 21       | 0.17          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 21       | 0.17          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 34       | 0.17          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 34       | 0.17          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 34       | 0.17          |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 4        | 0.17          |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 4        | 0.17          |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 4        | 0.17          |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 11       | 0.17          |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 11       | 0.17          |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 11       | 0.17          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 16       | 0.17          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 16       | 0.17          |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 16       | 0.17          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 23       | 0.17          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 23       | 0.17          |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 23       | 0.17          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 31       | 0.17          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 31       | 0.17          |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 31       | 0.17          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 35       | 0.17          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 35       | 0.17          |

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| Key      | Atom-1          | Atom-2       | Model ID | Violation (Å) |
|----------|-----------------|--------------|----------|---------------|
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H | 35       | 0.17          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H | 39       | 0.17          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H | 39       | 0.17          |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H | 39       | 0.17          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H | 40       | 0.17          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H | 40       | 0.17          |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H | 40       | 0.17          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 1        | 0.17          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 1        | 0.17          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 1        | 0.17          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 2        | 0.17          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 2        | 0.17          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 2        | 0.17          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 7        | 0.17          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 7        | 0.17          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 7        | 0.17          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 10       | 0.17          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 10       | 0.17          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 10       | 0.17          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 16       | 0.17          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 16       | 0.17          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 16       | 0.17          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H | 20       | 0.17          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H | 20       | 0.17          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H | 20       | 0.17          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 1        | 0.17          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 1        | 0.17          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 1        | 0.17          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 5        | 0.17          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 5        | 0.17          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 5        | 0.17          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 8        | 0.17          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 8        | 0.17          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 8        | 0.17          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 9        | 0.17          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 9        | 0.17          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 9        | 0.17          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 10       | 0.17          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 10       | 0.17          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 10       | 0.17          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 13       | 0.17          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 13       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H    | 13       | 0.17          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H    | 15       | 0.17          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H    | 15       | 0.17          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H    | 15       | 0.17          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H    | 17       | 0.17          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H    | 17       | 0.17          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H    | 17       | 0.17          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H    | 23       | 0.17          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H    | 23       | 0.17          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H    | 23       | 0.17          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H    | 28       | 0.17          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H    | 28       | 0.17          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H    | 28       | 0.17          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H    | 32       | 0.17          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H    | 32       | 0.17          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H    | 32       | 0.17          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H    | 34       | 0.17          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H    | 34       | 0.17          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H    | 34       | 0.17          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H    | 39       | 0.17          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H    | 39       | 0.17          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H    | 39       | 0.17          |
| (1,1401) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H    | 2        | 0.17          |
| (1,1401) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H    | 2        | 0.17          |
| (1,1401) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H    | 2        | 0.17          |
| (1,1401) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H    | 17       | 0.17          |
| (1,1401) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H    | 17       | 0.17          |
| (1,1401) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H    | 17       | 0.17          |
| (1,1401) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H    | 22       | 0.17          |
| (1,1401) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H    | 22       | 0.17          |
| (1,1401) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H    | 22       | 0.17          |
| (1,1401) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H    | 26       | 0.17          |
| (1,1401) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H    | 26       | 0.17          |
| (1,1401) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H    | 26       | 0.17          |
| (1,1401) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H    | 29       | 0.17          |
| (1,1401) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H    | 29       | 0.17          |
| (1,1401) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H    | 29       | 0.17          |
| (1,1400) | 1:95:A:ALA:HB1  | 1:16:A:ILE:HG12 | 20       | 0.17          |
| (1,1400) | 1:95:A:ALA:HB2  | 1:16:A:ILE:HG12 | 20       | 0.17          |
| (1,1400) | 1:95:A:ALA:HB3  | 1:16:A:ILE:HG12 | 20       | 0.17          |
| (1,1400) | 1:95:A:ALA:HB1  | 1:16:A:ILE:HG12 | 21       | 0.17          |
| (1,1400) | 1:95:A:ALA:HB2  | 1:16:A:ILE:HG12 | 21       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1400) | 1:95:A:ALA:HB3  | 1:16:A:ILE:HG12 | 21       | 0.17          |
| (1,1400) | 1:95:A:ALA:HB1  | 1:16:A:ILE:HG12 | 35       | 0.17          |
| (1,1400) | 1:95:A:ALA:HB2  | 1:16:A:ILE:HG12 | 35       | 0.17          |
| (1,1400) | 1:95:A:ALA:HB3  | 1:16:A:ILE:HG12 | 35       | 0.17          |
| (1,1387) | 1:91:A:ALA:HB1  | 1:12:A:PHE:HZ   | 27       | 0.17          |
| (1,1387) | 1:91:A:ALA:HB2  | 1:12:A:PHE:HZ   | 27       | 0.17          |
| (1,1387) | 1:91:A:ALA:HB3  | 1:12:A:PHE:HZ   | 27       | 0.17          |
| (1,1384) | 1:91:A:ALA:HB1  | 1:83:A:ALA:HB1  | 3        | 0.17          |
| (1,1384) | 1:91:A:ALA:HB1  | 1:83:A:ALA:HB2  | 3        | 0.17          |
| (1,1384) | 1:91:A:ALA:HB1  | 1:83:A:ALA:HB3  | 3        | 0.17          |
| (1,1384) | 1:91:A:ALA:HB2  | 1:83:A:ALA:HB1  | 3        | 0.17          |
| (1,1384) | 1:91:A:ALA:HB2  | 1:83:A:ALA:HB2  | 3        | 0.17          |
| (1,1384) | 1:91:A:ALA:HB2  | 1:83:A:ALA:HB3  | 3        | 0.17          |
| (1,1384) | 1:91:A:ALA:HB3  | 1:83:A:ALA:HB1  | 3        | 0.17          |
| (1,1384) | 1:91:A:ALA:HB3  | 1:83:A:ALA:HB2  | 3        | 0.17          |
| (1,1384) | 1:91:A:ALA:HB3  | 1:83:A:ALA:HB3  | 3        | 0.17          |
| (1,1379) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB1  | 3        | 0.17          |
| (1,1379) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB2  | 3        | 0.17          |
| (1,1379) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB3  | 3        | 0.17          |
| (1,1379) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB1  | 3        | 0.17          |
| (1,1379) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB2  | 3        | 0.17          |
| (1,1379) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB3  | 3        | 0.17          |
| (1,1379) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB1  | 3        | 0.17          |
| (1,1379) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB2  | 3        | 0.17          |
| (1,1379) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB3  | 3        | 0.17          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 13       | 0.17          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 22       | 0.17          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 26       | 0.17          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 31       | 0.17          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 38       | 0.17          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 2        | 0.17          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 2        | 0.17          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 2        | 0.17          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 4        | 0.17          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 4        | 0.17          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 4        | 0.17          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 8        | 0.17          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 8        | 0.17          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 8        | 0.17          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 10       | 0.17          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 10       | 0.17          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 10       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 12       | 0.17          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 12       | 0.17          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 12       | 0.17          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 27       | 0.17          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 27       | 0.17          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 27       | 0.17          |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 2        | 0.17          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 3        | 0.17          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 3        | 0.17          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 3        | 0.17          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 14       | 0.17          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 14       | 0.17          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 14       | 0.17          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 15       | 0.17          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 15       | 0.17          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 15       | 0.17          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 18       | 0.17          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 18       | 0.17          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 18       | 0.17          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 26       | 0.17          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 26       | 0.17          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 26       | 0.17          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 40       | 0.17          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 40       | 0.17          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 40       | 0.17          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 3        | 0.17          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 3        | 0.17          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 3        | 0.17          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 14       | 0.17          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 14       | 0.17          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 14       | 0.17          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 15       | 0.17          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 15       | 0.17          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 15       | 0.17          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 18       | 0.17          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 18       | 0.17          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 18       | 0.17          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 26       | 0.17          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 26       | 0.17          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 26       | 0.17          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 40       | 0.17          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 40       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 40       | 0.17          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 14       | 0.17          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 14       | 0.17          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 14       | 0.17          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 14       | 0.17          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 14       | 0.17          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 14       | 0.17          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 14       | 0.17          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 14       | 0.17          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 14       | 0.17          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 6        | 0.17          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 6        | 0.17          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 6        | 0.17          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 19       | 0.17          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 19       | 0.17          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 19       | 0.17          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 20       | 0.17          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 20       | 0.17          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 20       | 0.17          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 6        | 0.17          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 6        | 0.17          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 6        | 0.17          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 19       | 0.17          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 19       | 0.17          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 19       | 0.17          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 20       | 0.17          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 20       | 0.17          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 20       | 0.17          |
| (1,1257) | 1:67:A:THR:HG21 | 1:26:A:SER:HB2  | 1        | 0.17          |
| (1,1257) | 1:67:A:THR:HG22 | 1:26:A:SER:HB2  | 1        | 0.17          |
| (1,1257) | 1:67:A:THR:HG23 | 1:26:A:SER:HB2  | 1        | 0.17          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 5        | 0.17          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 5        | 0.17          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 5        | 0.17          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 23       | 0.17          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 23       | 0.17          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 23       | 0.17          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 34       | 0.17          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 34       | 0.17          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 34       | 0.17          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 36       | 0.17          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 36       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 36       | 0.17          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 13       | 0.17          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 13       | 0.17          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 13       | 0.17          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 15       | 0.17          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 15       | 0.17          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 15       | 0.17          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 20       | 0.17          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 20       | 0.17          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 20       | 0.17          |
| (1,1239) | 1:13:A:THR:HG21 | 1:34:A:SER:H    | 27       | 0.17          |
| (1,1239) | 1:13:A:THR:HG22 | 1:34:A:SER:H    | 27       | 0.17          |
| (1,1239) | 1:13:A:THR:HG23 | 1:34:A:SER:H    | 27       | 0.17          |
| (1,1236) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3  | 24       | 0.17          |
| (1,1236) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3  | 24       | 0.17          |
| (1,1236) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3  | 24       | 0.17          |
| (1,1226) | 1:101:A:LEU:H   | 1:22:A:SER:HA   | 9        | 0.17          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 3        | 0.17          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 6        | 0.17          |
| (1,1191) | 1:25:A:GLN:HE22 | 1:25:A:GLN:HB3  | 7        | 0.17          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 18       | 0.17          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 18       | 0.17          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 18       | 0.17          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 19       | 0.17          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 19       | 0.17          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 19       | 0.17          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 20       | 0.17          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 20       | 0.17          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 20       | 0.17          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 23       | 0.17          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 23       | 0.17          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 23       | 0.17          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 25       | 0.17          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 25       | 0.17          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 25       | 0.17          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 27       | 0.17          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 27       | 0.17          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 27       | 0.17          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 30       | 0.17          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 30       | 0.17          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 30       | 0.17          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 35       | 0.17          |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1190) | 1:22:A:SER:H  | 1:21:A:VAL:HG22 | 35       | 0.17          |
| (1,1190) | 1:22:A:SER:H  | 1:21:A:VAL:HG23 | 35       | 0.17          |
| (1,1190) | 1:22:A:SER:H  | 1:21:A:VAL:HG21 | 36       | 0.17          |
| (1,1190) | 1:22:A:SER:H  | 1:21:A:VAL:HG22 | 36       | 0.17          |
| (1,1190) | 1:22:A:SER:H  | 1:21:A:VAL:HG23 | 36       | 0.17          |
| (1,1190) | 1:22:A:SER:H  | 1:21:A:VAL:HG21 | 37       | 0.17          |
| (1,1190) | 1:22:A:SER:H  | 1:21:A:VAL:HG22 | 37       | 0.17          |
| (1,1190) | 1:22:A:SER:H  | 1:21:A:VAL:HG23 | 37       | 0.17          |
| (1,1185) | 1:21:A:VAL:H  | 1:100:A:GLU:HB3 | 11       | 0.17          |
| (1,1185) | 1:21:A:VAL:H  | 1:100:A:GLU:HB3 | 27       | 0.17          |
| (1,1185) | 1:21:A:VAL:H  | 1:100:A:GLU:HB3 | 30       | 0.17          |
| (1,1177) | 1:100:A:GLU:H | 1:21:A:VAL:HG11 | 7        | 0.17          |
| (1,1177) | 1:100:A:GLU:H | 1:21:A:VAL:HG12 | 7        | 0.17          |
| (1,1177) | 1:100:A:GLU:H | 1:21:A:VAL:HG13 | 7        | 0.17          |
| (1,1176) | 1:47:A:THR:H  | 1:44:A:LYS:HB3  | 11       | 0.17          |
| (1,1176) | 1:47:A:THR:H  | 1:44:A:LYS:HB3  | 18       | 0.17          |
| (1,1174) | 1:91:A:ALA:H  | 1:84:A:ARG:HA   | 4        | 0.17          |
| (1,1174) | 1:91:A:ALA:H  | 1:84:A:ARG:HA   | 8        | 0.17          |
| (1,1169) | 1:14:A:LYS:H  | 1:14:A:LYS:HD2  | 7        | 0.17          |
| (1,1163) | 1:75:A:ASP:H  | 1:74:A:ASP:HB2  | 7        | 0.17          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 6        | 0.17          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 6        | 0.17          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 14       | 0.17          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 14       | 0.17          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 16       | 0.17          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 16       | 0.17          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 22       | 0.17          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 22       | 0.17          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 25       | 0.17          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 25       | 0.17          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 28       | 0.17          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 28       | 0.17          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 31       | 0.17          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 31       | 0.17          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 32       | 0.17          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 32       | 0.17          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 33       | 0.17          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 33       | 0.17          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 34       | 0.17          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 34       | 0.17          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 37       | 0.17          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 37       | 0.17          |

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| Key      | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|----------|---------------|----------------|----------|---------------|
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1 | 39       | 0.17          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2 | 39       | 0.17          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1 | 40       | 0.17          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2 | 40       | 0.17          |
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 2        | 0.17          |
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 16       | 0.17          |
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 24       | 0.17          |
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 29       | 0.17          |
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H  | 33       | 0.17          |
| (1,1125) | 1:78:A:VAL:H  | 1:44:A:LYS:HE2 | 2        | 0.17          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA  | 3        | 0.17          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA  | 6        | 0.17          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA  | 10       | 0.17          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA  | 11       | 0.17          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA  | 12       | 0.17          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA  | 14       | 0.17          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA  | 15       | 0.17          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA  | 18       | 0.17          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA  | 19       | 0.17          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA  | 36       | 0.17          |
| (1,1064) | 1:71:A:VAL:H  | 1:25:A:GLN:H   | 17       | 0.17          |
| (1,987)  | 1:12:A:PHE:H  | 1:11:A:GLN:HB2 | 38       | 0.17          |
| (1,967)  | 1:21:A:VAL:H  | 1:99:A:GLY:HA3 | 7        | 0.17          |
| (1,967)  | 1:21:A:VAL:H  | 1:99:A:GLY:HA3 | 15       | 0.17          |
| (1,967)  | 1:21:A:VAL:H  | 1:99:A:GLY:HA3 | 34       | 0.17          |
| (1,941)  | 1:34:A:SER:H  | 1:12:A:PHE:HA  | 15       | 0.17          |
| (1,941)  | 1:34:A:SER:H  | 1:12:A:PHE:HA  | 29       | 0.17          |
| (1,941)  | 1:34:A:SER:H  | 1:12:A:PHE:HA  | 32       | 0.17          |
| (1,941)  | 1:34:A:SER:H  | 1:12:A:PHE:HA  | 38       | 0.17          |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB  | 4        | 0.17          |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB  | 13       | 0.17          |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB  | 24       | 0.17          |
| (1,919)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB2 | 7        | 0.17          |
| (1,888)  | 1:80:A:SER:H  | 1:43:A:TYR:HB3 | 3        | 0.17          |
| (1,888)  | 1:80:A:SER:H  | 1:43:A:TYR:HB3 | 9        | 0.17          |
| (1,888)  | 1:80:A:SER:H  | 1:43:A:TYR:HB3 | 26       | 0.17          |
| (1,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3  | 5        | 0.17          |
| (1,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3  | 6        | 0.17          |
| (1,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3  | 9        | 0.17          |
| (1,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3  | 12       | 0.17          |
| (1,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3  | 13       | 0.17          |
| (1,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3  | 18       | 0.17          |

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| Key     | Atom-1       | Atom-2         | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (1,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2  | 23       | 0.17          |
| (1,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2  | 24       | 0.17          |
| (1,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2  | 25       | 0.17          |
| (1,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2  | 26       | 0.17          |
| (1,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2  | 28       | 0.17          |
| (1,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2  | 29       | 0.17          |
| (1,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2  | 37       | 0.17          |
| (1,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2  | 39       | 0.17          |
| (1,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA   | 7        | 0.17          |
| (1,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA   | 29       | 0.17          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1 | 1        | 0.17          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2 | 1        | 0.17          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3 | 1        | 0.17          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1 | 4        | 0.17          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2 | 4        | 0.17          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3 | 4        | 0.17          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1 | 8        | 0.17          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2 | 8        | 0.17          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3 | 8        | 0.17          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1 | 19       | 0.17          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2 | 19       | 0.17          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3 | 19       | 0.17          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1 | 27       | 0.17          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2 | 27       | 0.17          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3 | 27       | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 3        | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 4        | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 5        | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 6        | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 8        | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 9        | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 10       | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 11       | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 12       | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 13       | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 14       | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 16       | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 17       | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 18       | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 19       | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 20       | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 21       | 0.17          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 22       | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 23       | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 24       | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 25       | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 26       | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 27       | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 28       | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 29       | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 30       | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 31       | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 32       | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 33       | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 34       | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 35       | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 36       | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 37       | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 38       | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 39       | 0.17          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA   | 40       | 0.17          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 19       | 0.17          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 19       | 0.17          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 19       | 0.17          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 27       | 0.17          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 27       | 0.17          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 27       | 0.17          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 2        | 0.17          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 4        | 0.17          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 12       | 0.17          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 15       | 0.17          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 16       | 0.17          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 26       | 0.17          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 30       | 0.17          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2  | 31       | 0.17          |
| (1,786) | 1:6:A:THR:H  | 1:6:A:THR:HG21  | 33       | 0.17          |
| (1,786) | 1:6:A:THR:H  | 1:6:A:THR:HG22  | 33       | 0.17          |
| (1,786) | 1:6:A:THR:H  | 1:6:A:THR:HG23  | 33       | 0.17          |
| (1,783) | 1:74:A:ASP:H | 1:74:A:ASP:HB3  | 17       | 0.17          |
| (1,739) | 1:15:A:ARG:H | 1:14:A:LYS:HB2  | 5        | 0.17          |
| (1,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2  | 14       | 0.17          |
| (1,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2  | 20       | 0.17          |
| (1,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2  | 21       | 0.17          |
| (1,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2  | 26       | 0.17          |

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| Key     | Atom-1       | Atom-2         | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (1,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 32       | 0.17          |
| (1,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 36       | 0.17          |
| (1,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 40       | 0.17          |
| (1,684) | 1:23:A:GLU:H | 1:23:A:GLU:HB3 | 3        | 0.17          |
| (1,684) | 1:23:A:GLU:H | 1:23:A:GLU:HB3 | 5        | 0.17          |
| (1,684) | 1:23:A:GLU:H | 1:23:A:GLU:HB3 | 20       | 0.17          |
| (1,684) | 1:23:A:GLU:H | 1:23:A:GLU:HB3 | 23       | 0.17          |
| (1,684) | 1:23:A:GLU:H | 1:23:A:GLU:HB3 | 26       | 0.17          |
| (1,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 4        | 0.17          |
| (1,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 6        | 0.17          |
| (1,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 7        | 0.17          |
| (1,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 11       | 0.17          |
| (1,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 15       | 0.17          |
| (1,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 17       | 0.17          |
| (1,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 19       | 0.17          |
| (1,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 20       | 0.17          |
| (1,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 21       | 0.17          |
| (1,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 22       | 0.17          |
| (1,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 23       | 0.17          |
| (1,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 24       | 0.17          |
| (1,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 25       | 0.17          |
| (1,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 28       | 0.17          |
| (1,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 32       | 0.17          |
| (1,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 33       | 0.17          |
| (1,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 34       | 0.17          |
| (1,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 35       | 0.17          |
| (1,605) | 1:50:A:THR:H | 1:49:A:LEU:HB2 | 36       | 0.17          |
| (1,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 3        | 0.17          |
| (1,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 9        | 0.17          |
| (1,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 10       | 0.17          |
| (1,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 13       | 0.17          |
| (1,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 20       | 0.17          |
| (1,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 21       | 0.17          |
| (1,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 22       | 0.17          |
| (1,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 23       | 0.17          |
| (1,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 24       | 0.17          |
| (1,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 25       | 0.17          |
| (1,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 26       | 0.17          |
| (1,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 32       | 0.17          |
| (1,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 34       | 0.17          |
| (1,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 35       | 0.17          |
| (1,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 36       | 0.17          |

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| Key     | Atom-1       | Atom-2         | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (1,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 40       | 0.17          |
| (1,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1 | 4        | 0.17          |
| (1,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2 | 4        | 0.17          |
| (1,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1 | 30       | 0.17          |
| (1,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2 | 30       | 0.17          |
| (1,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1 | 32       | 0.17          |
| (1,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2 | 32       | 0.17          |
| (1,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA  | 37       | 0.17          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 3        | 0.17          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 10       | 0.17          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 17       | 0.17          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 22       | 0.17          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 23       | 0.17          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 25       | 0.17          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 26       | 0.17          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 29       | 0.17          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 30       | 0.17          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 32       | 0.17          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 33       | 0.17          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 35       | 0.17          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 36       | 0.17          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2 | 11       | 0.17          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2 | 20       | 0.17          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2 | 22       | 0.17          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2 | 23       | 0.17          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2 | 27       | 0.17          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H  | 17       | 0.17          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H  | 32       | 0.17          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H  | 37       | 0.17          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H  | 38       | 0.17          |
| (1,513) | 1:67:A:THR:H | 1:66:A:MET:HG3 | 6        | 0.17          |
| (1,513) | 1:67:A:THR:H | 1:66:A:MET:HG3 | 12       | 0.17          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2 | 1        | 0.17          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2 | 5        | 0.17          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2 | 9        | 0.17          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2 | 11       | 0.17          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2 | 13       | 0.17          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2 | 18       | 0.17          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2 | 23       | 0.17          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2 | 25       | 0.17          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2 | 27       | 0.17          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2 | 30       | 0.17          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 32       | 0.17          |
| (1,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 6        | 0.17          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 20       | 0.17          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 27       | 0.17          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 28       | 0.17          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 36       | 0.17          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 4        | 0.17          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 25       | 0.17          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 38       | 0.17          |
| (1,368) | 1:18:A:ASN:H | 1:17:A:GLN:HB3  | 37       | 0.17          |
| (1,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 2        | 0.17          |
| (1,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA   | 30       | 0.17          |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 17       | 0.17          |
| (1,274) | 1:66:A:MET:H | 1:66:A:MET:HG3  | 6        | 0.17          |
| (1,274) | 1:66:A:MET:H | 1:66:A:MET:HG3  | 21       | 0.17          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 6        | 0.17          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 6        | 0.17          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 6        | 0.17          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 19       | 0.17          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 19       | 0.17          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 19       | 0.17          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 20       | 0.17          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 20       | 0.17          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 20       | 0.17          |
| (1,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 4        | 0.17          |
| (1,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 7        | 0.17          |
| (1,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 15       | 0.17          |
| (1,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 17       | 0.17          |
| (1,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 18       | 0.17          |
| (1,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 20       | 0.17          |
| (1,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 25       | 0.17          |
| (1,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 26       | 0.17          |
| (1,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 30       | 0.17          |
| (1,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 32       | 0.17          |
| (1,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 34       | 0.17          |
| (1,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 37       | 0.17          |
| (1,235) | 1:13:A:THR:H | 1:12:A:PHE:HB2  | 40       | 0.17          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1  | 4        | 0.17          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2  | 4        | 0.17          |
| (1,201) | 1:90:A:GLU:H | 1:89:A:GLY:HA2  | 26       | 0.17          |
| (1,201) | 1:90:A:GLU:H | 1:89:A:GLY:HA2  | 33       | 0.17          |
| (1,201) | 1:90:A:GLU:H | 1:89:A:GLY:HA2  | 36       | 0.17          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,148) | 1:45:A:GLY:H  | 1:46:A:PRO:HD2  | 33       | 0.17          |
| (1,142) | 1:101:A:LEU:H | 1:100:A:GLU:HB2 | 22       | 0.17          |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 2        | 0.17          |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 16       | 0.17          |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 24       | 0.17          |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 29       | 0.17          |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 33       | 0.17          |
| (1,133) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 8        | 0.17          |
| (1,133) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 37       | 0.17          |
| (1,133) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 38       | 0.17          |
| (1,129) | 1:39:A:ILE:H  | 1:39:A:ILE:HA   | 24       | 0.17          |
| (1,129) | 1:39:A:ILE:H  | 1:39:A:ILE:HA   | 36       | 0.17          |
| (1,100) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 11       | 0.17          |
| (1,100) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 14       | 0.17          |
| (1,100) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 16       | 0.17          |
| (1,100) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 24       | 0.17          |
| (1,100) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 29       | 0.17          |
| (1,100) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 37       | 0.17          |
| (1,70)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 3        | 0.17          |
| (1,70)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 4        | 0.17          |
| (1,70)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 6        | 0.17          |
| (1,70)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 7        | 0.17          |
| (1,70)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 12       | 0.17          |
| (1,70)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 14       | 0.17          |
| (1,70)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 19       | 0.17          |
| (1,70)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 23       | 0.17          |
| (1,70)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 25       | 0.17          |
| (1,70)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 26       | 0.17          |
| (1,70)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 28       | 0.17          |
| (1,70)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 29       | 0.17          |
| (1,70)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 31       | 0.17          |
| (1,70)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 32       | 0.17          |
| (1,70)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 33       | 0.17          |
| (1,70)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 34       | 0.17          |
| (1,70)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 35       | 0.17          |
| (1,70)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 36       | 0.17          |
| (1,70)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 40       | 0.17          |
| (1,57)  | 1:42:A:TRP:H  | 1:41:A:THR:HB   | 2        | 0.17          |
| (1,57)  | 1:42:A:TRP:H  | 1:41:A:THR:HB   | 5        | 0.17          |
| (1,57)  | 1:42:A:TRP:H  | 1:41:A:THR:HB   | 9        | 0.17          |
| (1,57)  | 1:42:A:TRP:H  | 1:41:A:THR:HB   | 16       | 0.17          |
| (1,57)  | 1:42:A:TRP:H  | 1:41:A:THR:HB   | 17       | 0.17          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,57)   | 1:42:A:TRP:H   | 1:41:A:THR:HB  | 18       | 0.17          |
| (1,57)   | 1:42:A:TRP:H   | 1:41:A:THR:HB  | 19       | 0.17          |
| (1,57)   | 1:42:A:TRP:H   | 1:41:A:THR:HB  | 25       | 0.17          |
| (1,57)   | 1:42:A:TRP:H   | 1:41:A:THR:HB  | 26       | 0.17          |
| (1,57)   | 1:42:A:TRP:H   | 1:41:A:THR:HB  | 28       | 0.17          |
| (1,57)   | 1:42:A:TRP:H   | 1:41:A:THR:HB  | 29       | 0.17          |
| (1,57)   | 1:42:A:TRP:H   | 1:41:A:THR:HB  | 30       | 0.17          |
| (1,57)   | 1:42:A:TRP:H   | 1:41:A:THR:HB  | 32       | 0.17          |
| (1,57)   | 1:42:A:TRP:H   | 1:41:A:THR:HB  | 34       | 0.17          |
| (1,57)   | 1:42:A:TRP:H   | 1:41:A:THR:HB  | 37       | 0.17          |
| (1,57)   | 1:42:A:TRP:H   | 1:41:A:THR:HB  | 38       | 0.17          |
| (1,57)   | 1:42:A:TRP:H   | 1:41:A:THR:HB  | 39       | 0.17          |
| (1,57)   | 1:42:A:TRP:H   | 1:41:A:THR:HB  | 40       | 0.17          |
| (1,49)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2 | 1        | 0.17          |
| (1,49)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2 | 6        | 0.17          |
| (1,49)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2 | 10       | 0.17          |
| (1,49)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2 | 12       | 0.17          |
| (1,49)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2 | 16       | 0.17          |
| (1,49)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2 | 18       | 0.17          |
| (1,49)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2 | 22       | 0.17          |
| (1,49)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2 | 26       | 0.17          |
| (1,49)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2 | 35       | 0.17          |
| (1,49)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2 | 40       | 0.17          |
| (1,35)   | 1:88:A:ARG:H   | 1:88:A:ARG:HG2 | 6        | 0.17          |
| (1,35)   | 1:88:A:ARG:H   | 1:88:A:ARG:HG2 | 7        | 0.17          |
| (1,35)   | 1:88:A:ARG:H   | 1:88:A:ARG:HG2 | 12       | 0.17          |
| (1,35)   | 1:88:A:ARG:H   | 1:88:A:ARG:HG2 | 13       | 0.17          |
| (1,22)   | 1:89:A:GLY:H   | 1:85:A:LEU:H   | 4        | 0.17          |
| (1,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3 | 29       | 0.17          |
| (1,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3 | 31       | 0.17          |
| (1,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3 | 33       | 0.17          |
| (1,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3 | 36       | 0.17          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3 | 3        | 0.16          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3 | 3        | 0.16          |
| (3,3217) | 1:69:A:HIS:HE1 | 1:67:A:THR:HB  | 23       | 0.16          |
| (3,3217) | 1:69:A:HIS:HE1 | 1:67:A:THR:HB  | 25       | 0.16          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1 | 8        | 0.16          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2 | 8        | 0.16          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1 | 14       | 0.16          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2 | 14       | 0.16          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1 | 39       | 0.16          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2 | 39       | 0.16          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 6        | 0.16          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 6        | 0.16          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 6        | 0.16          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 6        | 0.16          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 6        | 0.16          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 6        | 0.16          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 35       | 0.16          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 35       | 0.16          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 35       | 0.16          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 35       | 0.16          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 35       | 0.16          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 35       | 0.16          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 39       | 0.16          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 39       | 0.16          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 39       | 0.16          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 39       | 0.16          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 39       | 0.16          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 39       | 0.16          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 4        | 0.16          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 4        | 0.16          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 4        | 0.16          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 4        | 0.16          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 19       | 0.16          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 19       | 0.16          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 19       | 0.16          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 19       | 0.16          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 24       | 0.16          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 24       | 0.16          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 24       | 0.16          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 24       | 0.16          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 29       | 0.16          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 29       | 0.16          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 29       | 0.16          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 29       | 0.16          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 19       | 0.16          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 24       | 0.16          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 35       | 0.16          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 38       | 0.16          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 39       | 0.16          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 29       | 0.16          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 29       | 0.16          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 29       | 0.16          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,3164) | 1:42:A:TRP:HD1 | 1:41:A:THR:HA  | 16       | 0.16          |
| (3,3143) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3 | 25       | 0.16          |
| (3,3143) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3 | 25       | 0.16          |
| (3,3143) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3 | 30       | 0.16          |
| (3,3143) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3 | 30       | 0.16          |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 4        | 0.16          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 4        | 0.16          |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 18       | 0.16          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 18       | 0.16          |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 25       | 0.16          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 25       | 0.16          |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 32       | 0.16          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 32       | 0.16          |
| (3,3137) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3 | 14       | 0.16          |
| (3,3137) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3 | 14       | 0.16          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 2        | 0.16          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 2        | 0.16          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 8        | 0.16          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 8        | 0.16          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 16       | 0.16          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 16       | 0.16          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 23       | 0.16          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 23       | 0.16          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 32       | 0.16          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 32       | 0.16          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 38       | 0.16          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 38       | 0.16          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 39       | 0.16          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 39       | 0.16          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 2        | 0.16          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 2        | 0.16          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 8        | 0.16          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 8        | 0.16          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 16       | 0.16          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 16       | 0.16          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 23       | 0.16          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 23       | 0.16          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 32       | 0.16          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 32       | 0.16          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 38       | 0.16          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 38       | 0.16          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 39       | 0.16          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 39       | 0.16          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 9        | 0.16          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 9        | 0.16          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 9        | 0.16          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 9        | 0.16          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 9        | 0.16          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 9        | 0.16          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 13       | 0.16          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 13       | 0.16          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 13       | 0.16          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 13       | 0.16          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 13       | 0.16          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 13       | 0.16          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 17       | 0.16          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 17       | 0.16          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 17       | 0.16          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 17       | 0.16          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 17       | 0.16          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 17       | 0.16          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 26       | 0.16          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 26       | 0.16          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 26       | 0.16          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 26       | 0.16          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 26       | 0.16          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 26       | 0.16          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 35       | 0.16          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 35       | 0.16          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 35       | 0.16          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 35       | 0.16          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 35       | 0.16          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 35       | 0.16          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 2        | 0.16          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 2        | 0.16          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 2        | 0.16          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 2        | 0.16          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 2        | 0.16          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 2        | 0.16          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 8        | 0.16          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 8        | 0.16          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 8        | 0.16          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 8        | 0.16          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 8        | 0.16          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 8        | 0.16          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 9        | 0.16          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 9        | 0.16          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 9        | 0.16          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 9        | 0.16          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 9        | 0.16          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 9        | 0.16          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 13       | 0.16          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 13       | 0.16          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 13       | 0.16          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 13       | 0.16          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 13       | 0.16          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 13       | 0.16          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 18       | 0.16          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 18       | 0.16          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 18       | 0.16          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 18       | 0.16          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 18       | 0.16          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 18       | 0.16          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 32       | 0.16          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 32       | 0.16          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 32       | 0.16          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 32       | 0.16          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 19       | 0.16          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 19       | 0.16          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 19       | 0.16          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 19       | 0.16          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 19       | 0.16          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 19       | 0.16          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 29       | 0.16          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 29       | 0.16          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 29       | 0.16          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 29       | 0.16          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 29       | 0.16          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 29       | 0.16          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 9        | 0.16          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 10       | 0.16          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 13       | 0.16          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 21       | 0.16          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 22       | 0.16          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 23       | 0.16          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 24       | 0.16          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 25       | 0.16          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 26       | 0.16          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 27       | 0.16          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 28       | 0.16          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 30       | 0.16          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 31       | 0.16          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 32       | 0.16          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 35       | 0.16          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 36       | 0.16          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 38       | 0.16          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 39       | 0.16          |
| (3,3094) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 40       | 0.16          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 8        | 0.16          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 8        | 0.16          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 8        | 0.16          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 29       | 0.16          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 29       | 0.16          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 29       | 0.16          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 32       | 0.16          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 32       | 0.16          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 37       | 0.16          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 37       | 0.16          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 3        | 0.16          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 18       | 0.16          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 22       | 0.16          |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 2        | 0.16          |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 2        | 0.16          |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 3        | 0.16          |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 3        | 0.16          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 1        | 0.16          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 1        | 0.16          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 1        | 0.16          |
| (3,3019) | 1:30:A:GLU:HB2 | 1:14:A:LYS:HE2  | 14       | 0.16          |
| (3,3019) | 1:30:A:GLU:HB2 | 1:14:A:LYS:HE2  | 35       | 0.16          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 14       | 0.16          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 14       | 0.16          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 14       | 0.16          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 29       | 0.16          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 29       | 0.16          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 29       | 0.16          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 30       | 0.16          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 30       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG23 | 30       | 0.16          |
| (3,3004) | 1:15:A:ARG:HG2  | 1:93:A:SER:HB3  | 14       | 0.16          |
| (3,3004) | 1:15:A:ARG:HG2  | 1:93:A:SER:HB3  | 24       | 0.16          |
| (3,2970) | 1:44:A:LYS:HE2  | 1:44:A:LYS:HG3  | 20       | 0.16          |
| (3,2944) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD1  | 25       | 0.16          |
| (3,2944) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD2  | 25       | 0.16          |
| (3,2944) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD1  | 30       | 0.16          |
| (3,2944) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD2  | 30       | 0.16          |
| (3,2938) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 15       | 0.16          |
| (3,2938) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 29       | 0.16          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 13       | 0.16          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 20       | 0.16          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 27       | 0.16          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 28       | 0.16          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 29       | 0.16          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 1        | 0.16          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 3        | 0.16          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 5        | 0.16          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 7        | 0.16          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 8        | 0.16          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 15       | 0.16          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 16       | 0.16          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 26       | 0.16          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 29       | 0.16          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 36       | 0.16          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 4        | 0.16          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 6        | 0.16          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 15       | 0.16          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 29       | 0.16          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 33       | 0.16          |
| (3,2761) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 1        | 0.16          |
| (3,2761) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 5        | 0.16          |
| (3,2761) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 9        | 0.16          |
| (3,2761) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 10       | 0.16          |
| (3,2761) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 33       | 0.16          |
| (3,2761) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 37       | 0.16          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H    | 8        | 0.16          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H    | 13       | 0.16          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H    | 15       | 0.16          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H    | 22       | 0.16          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H    | 23       | 0.16          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H    | 25       | 0.16          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,2727) | 1:76:A:GLU:HB2 | 1:77:A:GLY:H    | 26       | 0.16          |
| (3,2727) | 1:76:A:GLU:HB2 | 1:77:A:GLY:H    | 29       | 0.16          |
| (3,2727) | 1:76:A:GLU:HB2 | 1:77:A:GLY:H    | 30       | 0.16          |
| (3,2727) | 1:76:A:GLU:HB2 | 1:77:A:GLY:H    | 35       | 0.16          |
| (3,2727) | 1:76:A:GLU:HB2 | 1:77:A:GLY:H    | 38       | 0.16          |
| (3,2727) | 1:76:A:GLU:HB2 | 1:77:A:GLY:H    | 39       | 0.16          |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 4        | 0.16          |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 5        | 0.16          |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 18       | 0.16          |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 19       | 0.16          |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 27       | 0.16          |
| (3,2679) | 1:25:A:GLN:HG3 | 1:26:A:SER:H    | 4        | 0.16          |
| (3,2679) | 1:25:A:GLN:HG3 | 1:26:A:SER:H    | 10       | 0.16          |
| (3,2679) | 1:25:A:GLN:HG3 | 1:26:A:SER:H    | 11       | 0.16          |
| (3,2679) | 1:25:A:GLN:HG3 | 1:26:A:SER:H    | 12       | 0.16          |
| (3,2679) | 1:25:A:GLN:HG3 | 1:26:A:SER:H    | 28       | 0.16          |
| (3,2679) | 1:25:A:GLN:HG3 | 1:26:A:SER:H    | 30       | 0.16          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 6        | 0.16          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 6        | 0.16          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 6        | 0.16          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 7        | 0.16          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 7        | 0.16          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 7        | 0.16          |
| (3,2602) | 1:36:A:ASP:HB2 | 1:37:A:ASP:H    | 31       | 0.16          |
| (3,2554) | 1:92:A:ARG:HA  | 1:83:A:ALA:H    | 18       | 0.16          |
| (3,2554) | 1:92:A:ARG:HA  | 1:83:A:ALA:H    | 28       | 0.16          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA   | 16       | 0.16          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA    | 11       | 0.16          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3   | 3        | 0.16          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3   | 4        | 0.16          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3   | 8        | 0.16          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3   | 14       | 0.16          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3   | 16       | 0.16          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3   | 17       | 0.16          |
| (3,2478) | 1:4:A:PRO:HG3  | 1:4:A:PRO:HG2   | 1        | 0.16          |
| (3,2478) | 1:4:A:PRO:HG3  | 1:4:A:PRO:HG2   | 4        | 0.16          |
| (3,2478) | 1:4:A:PRO:HG3  | 1:4:A:PRO:HG2   | 9        | 0.16          |
| (3,2478) | 1:4:A:PRO:HG3  | 1:4:A:PRO:HG2   | 10       | 0.16          |
| (3,2478) | 1:4:A:PRO:HG3  | 1:4:A:PRO:HG2   | 12       | 0.16          |
| (3,2478) | 1:4:A:PRO:HG3  | 1:4:A:PRO:HG2   | 15       | 0.16          |
| (3,2478) | 1:4:A:PRO:HG3  | 1:4:A:PRO:HG2   | 16       | 0.16          |
| (3,2478) | 1:4:A:PRO:HG3  | 1:4:A:PRO:HG2   | 17       | 0.16          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,2478) | 1:4:A:PRO:HG3  | 1:4:A:PRO:HG2  | 18       | 0.16          |
| (3,2478) | 1:4:A:PRO:HG3  | 1:4:A:PRO:HG2  | 35       | 0.16          |
| (3,2477) | 1:4:A:PRO:HG2  | 1:4:A:PRO:HG3  | 1        | 0.16          |
| (3,2477) | 1:4:A:PRO:HG2  | 1:4:A:PRO:HG3  | 4        | 0.16          |
| (3,2477) | 1:4:A:PRO:HG2  | 1:4:A:PRO:HG3  | 9        | 0.16          |
| (3,2477) | 1:4:A:PRO:HG2  | 1:4:A:PRO:HG3  | 10       | 0.16          |
| (3,2477) | 1:4:A:PRO:HG2  | 1:4:A:PRO:HG3  | 12       | 0.16          |
| (3,2477) | 1:4:A:PRO:HG2  | 1:4:A:PRO:HG3  | 15       | 0.16          |
| (3,2477) | 1:4:A:PRO:HG2  | 1:4:A:PRO:HG3  | 16       | 0.16          |
| (3,2477) | 1:4:A:PRO:HG2  | 1:4:A:PRO:HG3  | 17       | 0.16          |
| (3,2477) | 1:4:A:PRO:HG2  | 1:4:A:PRO:HG3  | 18       | 0.16          |
| (3,2477) | 1:4:A:PRO:HG2  | 1:4:A:PRO:HG3  | 35       | 0.16          |
| (3,2463) | 1:4:A:PRO:HD3  | 1:3:A:ASP:HA   | 3        | 0.16          |
| (3,2434) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 19       | 0.16          |
| (3,2412) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 13       | 0.16          |
| (3,2412) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 31       | 0.16          |
| (3,2412) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 33       | 0.16          |
| (3,2412) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 35       | 0.16          |
| (3,2412) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 36       | 0.16          |
| (3,2406) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 9        | 0.16          |
| (3,2406) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 9        | 0.16          |
| (3,2406) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 9        | 0.16          |
| (3,2406) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 13       | 0.16          |
| (3,2406) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 13       | 0.16          |
| (3,2406) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 13       | 0.16          |
| (3,2406) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 14       | 0.16          |
| (3,2406) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 14       | 0.16          |
| (3,2406) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 14       | 0.16          |
| (3,2406) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 18       | 0.16          |
| (3,2406) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 18       | 0.16          |
| (3,2406) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 18       | 0.16          |
| (3,2406) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 27       | 0.16          |
| (3,2406) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 27       | 0.16          |
| (3,2406) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 27       | 0.16          |
| (3,2406) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 32       | 0.16          |
| (3,2406) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 32       | 0.16          |
| (3,2406) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 32       | 0.16          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 15       | 0.16          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 15       | 0.16          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 15       | 0.16          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 35       | 0.16          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 35       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2405) | 1:66:A:MET:HE3  | 1:29:A:PHE:HZ   | 35       | 0.16          |
| (3,2290) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 5        | 0.16          |
| (3,2290) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 13       | 0.16          |
| (3,2290) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 16       | 0.16          |
| (3,2290) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 38       | 0.16          |
| (3,2289) | 1:96:A:GLU:HG2  | 1:97:A:LEU:H    | 3        | 0.16          |
| (3,2289) | 1:96:A:GLU:HG2  | 1:97:A:LEU:H    | 5        | 0.16          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 14       | 0.16          |
| (3,2253) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 14       | 0.16          |
| (3,2218) | 1:56:A:ASN:HA   | 1:56:A:ASN:HD21 | 7        | 0.16          |
| (3,2173) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 8        | 0.16          |
| (3,2148) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 21       | 0.16          |
| (3,2102) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HA   | 24       | 0.16          |
| (3,2102) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HA   | 24       | 0.16          |
| (3,2102) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HA   | 24       | 0.16          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 5        | 0.16          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 5        | 0.16          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 5        | 0.16          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 27       | 0.16          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 27       | 0.16          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 27       | 0.16          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 37       | 0.16          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 37       | 0.16          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 37       | 0.16          |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD11 | 8        | 0.16          |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD12 | 8        | 0.16          |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD13 | 8        | 0.16          |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD11 | 8        | 0.16          |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD12 | 8        | 0.16          |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD13 | 8        | 0.16          |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD11 | 8        | 0.16          |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD12 | 8        | 0.16          |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD13 | 8        | 0.16          |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD11 | 13       | 0.16          |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD12 | 13       | 0.16          |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD13 | 13       | 0.16          |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD11 | 13       | 0.16          |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD12 | 13       | 0.16          |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD13 | 13       | 0.16          |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD11 | 13       | 0.16          |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD12 | 13       | 0.16          |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD13 | 13       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD11 | 18       | 0.16          |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD12 | 18       | 0.16          |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD13 | 18       | 0.16          |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD11 | 18       | 0.16          |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD12 | 18       | 0.16          |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD13 | 18       | 0.16          |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD11 | 18       | 0.16          |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD12 | 18       | 0.16          |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD13 | 18       | 0.16          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1  | 15       | 0.16          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2  | 15       | 0.16          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1  | 15       | 0.16          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2  | 15       | 0.16          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1  | 15       | 0.16          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2  | 15       | 0.16          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 9        | 0.16          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 9        | 0.16          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 9        | 0.16          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 26       | 0.16          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 26       | 0.16          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 26       | 0.16          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 32       | 0.16          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 32       | 0.16          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 32       | 0.16          |
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3  | 14       | 0.16          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3  | 14       | 0.16          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3  | 14       | 0.16          |
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3  | 29       | 0.16          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3  | 29       | 0.16          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3  | 29       | 0.16          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1  | 20       | 0.16          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2  | 20       | 0.16          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1  | 20       | 0.16          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2  | 20       | 0.16          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1  | 20       | 0.16          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2  | 20       | 0.16          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1  | 35       | 0.16          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2  | 35       | 0.16          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1  | 35       | 0.16          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2  | 35       | 0.16          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1  | 35       | 0.16          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2  | 35       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 1        | 0.16          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 11       | 0.16          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 22       | 0.16          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 25       | 0.16          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 30       | 0.16          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 36       | 0.16          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 37       | 0.16          |
| (3,2008) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3  | 19       | 0.16          |
| (3,2008) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3  | 19       | 0.16          |
| (3,2008) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3  | 19       | 0.16          |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 11       | 0.16          |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 11       | 0.16          |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 11       | 0.16          |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 16       | 0.16          |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 16       | 0.16          |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 16       | 0.16          |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 35       | 0.16          |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 35       | 0.16          |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 35       | 0.16          |
| (3,1993) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 20       | 0.16          |
| (3,1993) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 20       | 0.16          |
| (3,1993) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 20       | 0.16          |
| (3,1969) | 1:36:A:ASP:HB3  | 1:62:A:ARG:HA   | 7        | 0.16          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 6        | 0.16          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 10       | 0.16          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 24       | 0.16          |
| (3,1955) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB1  | 5        | 0.16          |
| (3,1955) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB2  | 5        | 0.16          |
| (3,1955) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB3  | 5        | 0.16          |
| (3,1955) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB1  | 5        | 0.16          |
| (3,1955) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB2  | 5        | 0.16          |
| (3,1955) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB3  | 5        | 0.16          |
| (3,1955) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB1  | 5        | 0.16          |
| (3,1955) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB2  | 5        | 0.16          |
| (3,1955) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB3  | 5        | 0.16          |
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA   | 1        | 0.16          |
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA   | 1        | 0.16          |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA   | 1        | 0.16          |
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA   | 25       | 0.16          |
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA   | 25       | 0.16          |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA   | 25       | 0.16          |
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA   | 34       | 0.16          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA | 34       | 0.16          |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA | 34       | 0.16          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 1        | 0.16          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 1        | 0.16          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 1        | 0.16          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 2        | 0.16          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 2        | 0.16          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 2        | 0.16          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 3        | 0.16          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 3        | 0.16          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 3        | 0.16          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 4        | 0.16          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 4        | 0.16          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 4        | 0.16          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 7        | 0.16          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 7        | 0.16          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 7        | 0.16          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 9        | 0.16          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 9        | 0.16          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 9        | 0.16          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 11       | 0.16          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 11       | 0.16          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 11       | 0.16          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 16       | 0.16          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 16       | 0.16          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 16       | 0.16          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 19       | 0.16          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 19       | 0.16          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 19       | 0.16          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 24       | 0.16          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 24       | 0.16          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 24       | 0.16          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 27       | 0.16          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 27       | 0.16          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 27       | 0.16          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 35       | 0.16          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 35       | 0.16          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 35       | 0.16          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 36       | 0.16          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 36       | 0.16          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 36       | 0.16          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 38       | 0.16          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H   | 38       | 0.16          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H   | 38       | 0.16          |
| (3,1864) | 1:7:A:ALA:HB1   | 1:88:A:ARG:HA  | 8        | 0.16          |
| (3,1864) | 1:7:A:ALA:HB2   | 1:88:A:ARG:HA  | 8        | 0.16          |
| (3,1864) | 1:7:A:ALA:HB3   | 1:88:A:ARG:HA  | 8        | 0.16          |
| (3,1864) | 1:7:A:ALA:HB1   | 1:88:A:ARG:HA  | 32       | 0.16          |
| (3,1864) | 1:7:A:ALA:HB2   | 1:88:A:ARG:HA  | 32       | 0.16          |
| (3,1864) | 1:7:A:ALA:HB3   | 1:88:A:ARG:HA  | 32       | 0.16          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 2        | 0.16          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 2        | 0.16          |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 2        | 0.16          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 3        | 0.16          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 3        | 0.16          |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 3        | 0.16          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 11       | 0.16          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 11       | 0.16          |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 11       | 0.16          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 12       | 0.16          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 12       | 0.16          |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 12       | 0.16          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 16       | 0.16          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 16       | 0.16          |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 16       | 0.16          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 19       | 0.16          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 19       | 0.16          |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 19       | 0.16          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 22       | 0.16          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 22       | 0.16          |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 22       | 0.16          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 26       | 0.16          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 26       | 0.16          |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 26       | 0.16          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 27       | 0.16          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 27       | 0.16          |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 27       | 0.16          |
| (3,1813) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 4        | 0.16          |
| (3,1813) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 5        | 0.16          |
| (3,1813) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 6        | 0.16          |
| (3,1813) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 7        | 0.16          |
| (3,1813) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 8        | 0.16          |
| (3,1813) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 9        | 0.16          |
| (3,1813) | 1:98:A:LYS:HD3  | 1:98:A:LYS:HG3 | 10       | 0.16          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 13       | 0.16          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 19       | 0.16          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 21       | 0.16          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 22       | 0.16          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 23       | 0.16          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 25       | 0.16          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 29       | 0.16          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 30       | 0.16          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 31       | 0.16          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 32       | 0.16          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 36       | 0.16          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 38       | 0.16          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 39       | 0.16          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 40       | 0.16          |
| (3,1747) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H    | 1        | 0.16          |
| (3,1747) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H    | 5        | 0.16          |
| (3,1747) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H    | 8        | 0.16          |
| (3,1747) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H    | 10       | 0.16          |
| (3,1747) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H    | 13       | 0.16          |
| (3,1747) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H    | 16       | 0.16          |
| (3,1747) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H    | 20       | 0.16          |
| (3,1747) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H    | 37       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG11 | 14       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG12 | 14       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG13 | 14       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG11 | 14       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG12 | 14       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG13 | 14       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG11 | 14       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG12 | 14       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG13 | 14       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG11 | 21       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG12 | 21       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG13 | 21       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG11 | 21       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG12 | 21       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG13 | 21       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG11 | 21       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG12 | 21       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG13 | 21       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG11 | 38       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG12 | 38       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1721) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG13 | 38       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG11 | 38       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG12 | 38       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 38       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 38       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 38       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 38       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG11 | 39       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG12 | 39       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG13 | 39       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG11 | 39       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG12 | 39       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 39       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 39       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 39       | 0.16          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 39       | 0.16          |
| (3,1712) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 15       | 0.16          |
| (3,1712) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 15       | 0.16          |
| (3,1712) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 15       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 2        | 0.16          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 2        | 0.16          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 2        | 0.16          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 2        | 0.16          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 2        | 0.16          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 2        | 0.16          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 2        | 0.16          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 2        | 0.16          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 2        | 0.16          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 5        | 0.16          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 5        | 0.16          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 5        | 0.16          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 5        | 0.16          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 5        | 0.16          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 5        | 0.16          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 5        | 0.16          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 5        | 0.16          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 5        | 0.16          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 10       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 10       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 10       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 10       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 10       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 10       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 10       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 10       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 10       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 13       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 13       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 13       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 13       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 13       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 13       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 13       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 13       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 13       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 28       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 28       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 28       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 28       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 28       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 28       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 28       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 28       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 28       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 29       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 29       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 29       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 29       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 29       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 29       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 29       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 29       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 29       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 30       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 30       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 30       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 30       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 30       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 30       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 30       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 30       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 30       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 35       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 35       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 35       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 35       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 35       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 35       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 35       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 35       | 0.16          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 35       | 0.16          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 26       | 0.16          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 26       | 0.16          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 26       | 0.16          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 33       | 0.16          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 33       | 0.16          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 33       | 0.16          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 35       | 0.16          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 35       | 0.16          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 35       | 0.16          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 37       | 0.16          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 37       | 0.16          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 37       | 0.16          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 8        | 0.16          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 8        | 0.16          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 8        | 0.16          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 8        | 0.16          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 8        | 0.16          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 8        | 0.16          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 8        | 0.16          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 8        | 0.16          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 8        | 0.16          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 12       | 0.16          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 12       | 0.16          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 12       | 0.16          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 12       | 0.16          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 12       | 0.16          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 12       | 0.16          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 12       | 0.16          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 12       | 0.16          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 12       | 0.16          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 13       | 0.16          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 13       | 0.16          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 13       | 0.16          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 13       | 0.16          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 13       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 13       | 0.16          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 13       | 0.16          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 13       | 0.16          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 13       | 0.16          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 14       | 0.16          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 14       | 0.16          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 14       | 0.16          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 14       | 0.16          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 14       | 0.16          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 14       | 0.16          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 14       | 0.16          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 14       | 0.16          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 14       | 0.16          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 2        | 0.16          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 2        | 0.16          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 2        | 0.16          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 18       | 0.16          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 18       | 0.16          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 18       | 0.16          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 23       | 0.16          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 23       | 0.16          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 23       | 0.16          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 2        | 0.16          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 2        | 0.16          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 2        | 0.16          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 15       | 0.16          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 15       | 0.16          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 15       | 0.16          |
| (3,1623) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 32       | 0.16          |
| (3,1623) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 32       | 0.16          |
| (3,1623) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 32       | 0.16          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 29       | 0.16          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 29       | 0.16          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 29       | 0.16          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1  | 9        | 0.16          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2  | 9        | 0.16          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1  | 9        | 0.16          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2  | 9        | 0.16          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1  | 9        | 0.16          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2  | 9        | 0.16          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1  | 13       | 0.16          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2  | 13       | 0.16          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 13       | 0.16          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 13       | 0.16          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 13       | 0.16          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 13       | 0.16          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 17       | 0.16          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 17       | 0.16          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 17       | 0.16          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 17       | 0.16          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 17       | 0.16          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 17       | 0.16          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 26       | 0.16          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 26       | 0.16          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 26       | 0.16          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 26       | 0.16          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 26       | 0.16          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 26       | 0.16          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 35       | 0.16          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 35       | 0.16          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 35       | 0.16          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 35       | 0.16          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 35       | 0.16          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 35       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 13       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 13       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 13       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 13       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 13       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 13       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 17       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 17       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 17       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 17       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 17       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 17       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 19       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 19       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 19       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 19       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 19       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 19       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 20       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 20       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 20       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 20       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 20       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 20       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 27       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 27       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 27       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 27       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 27       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 27       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 30       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 30       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 30       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 30       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 30       | 0.16          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 30       | 0.16          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 1        | 0.16          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 1        | 0.16          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 1        | 0.16          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 2        | 0.16          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 2        | 0.16          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 2        | 0.16          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 13       | 0.16          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 13       | 0.16          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 13       | 0.16          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 25       | 0.16          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 25       | 0.16          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 25       | 0.16          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 33       | 0.16          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 33       | 0.16          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 33       | 0.16          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 38       | 0.16          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 38       | 0.16          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 38       | 0.16          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 1        | 0.16          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 1        | 0.16          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 1        | 0.16          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 2        | 0.16          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 2        | 0.16          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 2        | 0.16          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 4        | 0.16          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 4        | 0.16          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA  | 4        | 0.16          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA  | 5        | 0.16          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA  | 5        | 0.16          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA  | 5        | 0.16          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA  | 9        | 0.16          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA  | 9        | 0.16          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA  | 9        | 0.16          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA  | 18       | 0.16          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA  | 18       | 0.16          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA  | 18       | 0.16          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA  | 19       | 0.16          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA  | 19       | 0.16          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA  | 19       | 0.16          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA  | 20       | 0.16          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA  | 20       | 0.16          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA  | 20       | 0.16          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA  | 27       | 0.16          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA  | 27       | 0.16          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA  | 27       | 0.16          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA  | 31       | 0.16          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA  | 31       | 0.16          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA  | 31       | 0.16          |
| (3,1547) | 1:2:A:ILE:HG12  | 1:2:A:ILE:HA   | 8        | 0.16          |
| (3,1547) | 1:2:A:ILE:HG12  | 1:2:A:ILE:HA   | 10       | 0.16          |
| (3,1547) | 1:2:A:ILE:HG12  | 1:2:A:ILE:HA   | 14       | 0.16          |
| (3,1547) | 1:2:A:ILE:HG12  | 1:2:A:ILE:HA   | 17       | 0.16          |
| (3,1547) | 1:2:A:ILE:HG12  | 1:2:A:ILE:HA   | 30       | 0.16          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 13       | 0.16          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 13       | 0.16          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 13       | 0.16          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 19       | 0.16          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 19       | 0.16          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 19       | 0.16          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 36       | 0.16          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 36       | 0.16          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 36       | 0.16          |
| (3,1514) | 1:66:A:MET:HE1  | 1:42:A:TRP:HE1 | 29       | 0.16          |
| (3,1514) | 1:66:A:MET:HE2  | 1:42:A:TRP:HE1 | 29       | 0.16          |
| (3,1514) | 1:66:A:MET:HE3  | 1:42:A:TRP:HE1 | 29       | 0.16          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1 | 20       | 0.16          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2 | 20       | 0.16          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1 | 20       | 0.16          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 20       | 0.16          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 20       | 0.16          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 20       | 0.16          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 25       | 0.16          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 25       | 0.16          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 25       | 0.16          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 25       | 0.16          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 25       | 0.16          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 25       | 0.16          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 30       | 0.16          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 30       | 0.16          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 30       | 0.16          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 30       | 0.16          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 30       | 0.16          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 30       | 0.16          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 36       | 0.16          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 36       | 0.16          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 36       | 0.16          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 36       | 0.16          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 36       | 0.16          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 36       | 0.16          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 37       | 0.16          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 37       | 0.16          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 37       | 0.16          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 37       | 0.16          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 37       | 0.16          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 37       | 0.16          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 38       | 0.16          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 38       | 0.16          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 38       | 0.16          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 38       | 0.16          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 38       | 0.16          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 38       | 0.16          |
| (3,1512) | 1:66:A:MET:HE1 | 1:42:A:TRP:HZ3 | 9        | 0.16          |
| (3,1512) | 1:66:A:MET:HE2 | 1:42:A:TRP:HZ3 | 9        | 0.16          |
| (3,1512) | 1:66:A:MET:HE3 | 1:42:A:TRP:HZ3 | 9        | 0.16          |
| (3,1512) | 1:66:A:MET:HE1 | 1:42:A:TRP:HZ3 | 22       | 0.16          |
| (3,1512) | 1:66:A:MET:HE2 | 1:42:A:TRP:HZ3 | 22       | 0.16          |
| (3,1512) | 1:66:A:MET:HE3 | 1:42:A:TRP:HZ3 | 22       | 0.16          |
| (3,1512) | 1:66:A:MET:HE1 | 1:42:A:TRP:HZ3 | 36       | 0.16          |
| (3,1512) | 1:66:A:MET:HE2 | 1:42:A:TRP:HZ3 | 36       | 0.16          |
| (3,1512) | 1:66:A:MET:HE3 | 1:42:A:TRP:HZ3 | 36       | 0.16          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1504) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2 | 12       | 0.16          |
| (3,1504) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2 | 12       | 0.16          |
| (3,1504) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2 | 12       | 0.16          |
| (3,1504) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2 | 24       | 0.16          |
| (3,1504) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2 | 24       | 0.16          |
| (3,1504) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2 | 24       | 0.16          |
| (3,1504) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2 | 33       | 0.16          |
| (3,1504) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2 | 33       | 0.16          |
| (3,1504) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2 | 33       | 0.16          |
| (3,1504) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2 | 40       | 0.16          |
| (3,1504) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2 | 40       | 0.16          |
| (3,1504) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2 | 40       | 0.16          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 9        | 0.16          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 9        | 0.16          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 9        | 0.16          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 10       | 0.16          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 10       | 0.16          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 10       | 0.16          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 20       | 0.16          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 20       | 0.16          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 20       | 0.16          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 23       | 0.16          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 23       | 0.16          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 23       | 0.16          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 32       | 0.16          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 32       | 0.16          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 32       | 0.16          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 40       | 0.16          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 40       | 0.16          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 40       | 0.16          |
| (3,1474) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 29       | 0.16          |
| (3,1474) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 29       | 0.16          |
| (3,1474) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 29       | 0.16          |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 38       | 0.16          |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 38       | 0.16          |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 38       | 0.16          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 10       | 0.16          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 10       | 0.16          |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 10       | 0.16          |
| (3,1466) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H   | 4        | 0.16          |
| (3,1466) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H   | 4        | 0.16          |
| (3,1466) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H   | 4        | 0.16          |

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| Key      | Atom-1          | Atom-2       | Model ID | Violation (Å) |
|----------|-----------------|--------------|----------|---------------|
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 3        | 0.16          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 3        | 0.16          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 3        | 0.16          |
| (3,1414) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H | 12       | 0.16          |
| (3,1414) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H | 12       | 0.16          |
| (3,1414) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 12       | 0.16          |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H | 2        | 0.16          |
| (3,1407) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H | 2        | 0.16          |
| (3,1407) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H | 2        | 0.16          |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H | 3        | 0.16          |
| (3,1407) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H | 3        | 0.16          |
| (3,1407) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H | 3        | 0.16          |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H | 5        | 0.16          |
| (3,1407) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H | 5        | 0.16          |
| (3,1407) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H | 5        | 0.16          |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H | 12       | 0.16          |
| (3,1407) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H | 12       | 0.16          |
| (3,1407) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H | 12       | 0.16          |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H | 14       | 0.16          |
| (3,1407) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H | 14       | 0.16          |
| (3,1407) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H | 14       | 0.16          |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H | 24       | 0.16          |
| (3,1407) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H | 24       | 0.16          |
| (3,1407) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H | 24       | 0.16          |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H | 25       | 0.16          |
| (3,1407) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H | 25       | 0.16          |
| (3,1407) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H | 25       | 0.16          |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H | 30       | 0.16          |
| (3,1407) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H | 30       | 0.16          |
| (3,1407) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H | 30       | 0.16          |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H | 32       | 0.16          |
| (3,1407) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H | 32       | 0.16          |
| (3,1407) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H | 32       | 0.16          |
| (3,1405) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H | 5        | 0.16          |
| (3,1405) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H | 5        | 0.16          |
| (3,1405) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H | 5        | 0.16          |
| (3,1405) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H | 7        | 0.16          |
| (3,1405) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H | 7        | 0.16          |
| (3,1405) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H | 7        | 0.16          |
| (3,1405) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H | 11       | 0.16          |
| (3,1405) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H | 11       | 0.16          |
| (3,1405) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H | 11       | 0.16          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,1405) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H    | 15       | 0.16          |
| (3,1405) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H    | 15       | 0.16          |
| (3,1405) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 15       | 0.16          |
| (3,1405) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H    | 21       | 0.16          |
| (3,1405) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H    | 21       | 0.16          |
| (3,1405) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 21       | 0.16          |
| (3,1405) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H    | 31       | 0.16          |
| (3,1405) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H    | 31       | 0.16          |
| (3,1405) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 31       | 0.16          |
| (3,1405) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H    | 33       | 0.16          |
| (3,1405) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H    | 33       | 0.16          |
| (3,1405) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 33       | 0.16          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 8        | 0.16          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 8        | 0.16          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 8        | 0.16          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 18       | 0.16          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 18       | 0.16          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 18       | 0.16          |
| (3,1391) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ   | 17       | 0.16          |
| (3,1391) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ   | 17       | 0.16          |
| (3,1391) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ   | 17       | 0.16          |
| (3,1391) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ   | 32       | 0.16          |
| (3,1391) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ   | 32       | 0.16          |
| (3,1391) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ   | 32       | 0.16          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1  | 30       | 0.16          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2  | 30       | 0.16          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3  | 30       | 0.16          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1  | 30       | 0.16          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2  | 30       | 0.16          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3  | 30       | 0.16          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1  | 30       | 0.16          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2  | 30       | 0.16          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3  | 30       | 0.16          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1  | 36       | 0.16          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2  | 36       | 0.16          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3  | 36       | 0.16          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1  | 36       | 0.16          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2  | 36       | 0.16          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3  | 36       | 0.16          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1  | 36       | 0.16          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2  | 36       | 0.16          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3  | 36       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1383) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB1  | 30       | 0.16          |
| (3,1383) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB2  | 30       | 0.16          |
| (3,1383) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB3  | 30       | 0.16          |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB1  | 30       | 0.16          |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB2  | 30       | 0.16          |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB3  | 30       | 0.16          |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB1  | 30       | 0.16          |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB2  | 30       | 0.16          |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB3  | 30       | 0.16          |
| (3,1383) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB1  | 36       | 0.16          |
| (3,1383) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB2  | 36       | 0.16          |
| (3,1383) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB3  | 36       | 0.16          |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB1  | 36       | 0.16          |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB2  | 36       | 0.16          |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB3  | 36       | 0.16          |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB1  | 36       | 0.16          |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB2  | 36       | 0.16          |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB3  | 36       | 0.16          |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 1        | 0.16          |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 2        | 0.16          |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 4        | 0.16          |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 5        | 0.16          |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 10       | 0.16          |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 17       | 0.16          |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 20       | 0.16          |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 30       | 0.16          |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 35       | 0.16          |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 40       | 0.16          |
| (3,1364) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 16       | 0.16          |
| (3,1364) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 16       | 0.16          |
| (3,1364) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 16       | 0.16          |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 5        | 0.16          |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 11       | 0.16          |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 18       | 0.16          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 9        | 0.16          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 9        | 0.16          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 9        | 0.16          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 17       | 0.16          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 17       | 0.16          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 17       | 0.16          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 25       | 0.16          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 25       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 25       | 0.16          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 35       | 0.16          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 35       | 0.16          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 35       | 0.16          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 38       | 0.16          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 38       | 0.16          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 38       | 0.16          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 9        | 0.16          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 9        | 0.16          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 9        | 0.16          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 17       | 0.16          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 17       | 0.16          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 17       | 0.16          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 25       | 0.16          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 25       | 0.16          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 25       | 0.16          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 35       | 0.16          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 35       | 0.16          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 35       | 0.16          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 38       | 0.16          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 38       | 0.16          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 38       | 0.16          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 2        | 0.16          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 2        | 0.16          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 2        | 0.16          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 2        | 0.16          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 2        | 0.16          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 2        | 0.16          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 2        | 0.16          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 2        | 0.16          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 2        | 0.16          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 3        | 0.16          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 3        | 0.16          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 3        | 0.16          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 3        | 0.16          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 3        | 0.16          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 3        | 0.16          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 3        | 0.16          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 3        | 0.16          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 3        | 0.16          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 8        | 0.16          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 8        | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 8        | 0.16          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 8        | 0.16          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 8        | 0.16          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 8        | 0.16          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 8        | 0.16          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 8        | 0.16          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 8        | 0.16          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 10       | 0.16          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 10       | 0.16          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 10       | 0.16          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 10       | 0.16          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 10       | 0.16          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 10       | 0.16          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 10       | 0.16          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 10       | 0.16          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 10       | 0.16          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 15       | 0.16          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 15       | 0.16          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 15       | 0.16          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 15       | 0.16          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 15       | 0.16          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 15       | 0.16          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 15       | 0.16          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 15       | 0.16          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 15       | 0.16          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 19       | 0.16          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 19       | 0.16          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 19       | 0.16          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 19       | 0.16          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 19       | 0.16          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 19       | 0.16          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 19       | 0.16          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 19       | 0.16          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 19       | 0.16          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 26       | 0.16          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 26       | 0.16          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 26       | 0.16          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 26       | 0.16          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 26       | 0.16          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 26       | 0.16          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 26       | 0.16          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 26       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 26       | 0.16          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 27       | 0.16          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 27       | 0.16          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 27       | 0.16          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 27       | 0.16          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 27       | 0.16          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 27       | 0.16          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 27       | 0.16          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 27       | 0.16          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 27       | 0.16          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 6        | 0.16          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 6        | 0.16          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 6        | 0.16          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 28       | 0.16          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 28       | 0.16          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 28       | 0.16          |
| (3,1261) | 1:67:A:THR:HG21 | 1:26:A:SER:HB2  | 7        | 0.16          |
| (3,1261) | 1:67:A:THR:HG22 | 1:26:A:SER:HB2  | 7        | 0.16          |
| (3,1261) | 1:67:A:THR:HG23 | 1:26:A:SER:HB2  | 7        | 0.16          |
| (3,1261) | 1:67:A:THR:HG21 | 1:26:A:SER:HB2  | 31       | 0.16          |
| (3,1261) | 1:67:A:THR:HG22 | 1:26:A:SER:HB2  | 31       | 0.16          |
| (3,1261) | 1:67:A:THR:HG23 | 1:26:A:SER:HB2  | 31       | 0.16          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 1        | 0.16          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 1        | 0.16          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 1        | 0.16          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 8        | 0.16          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 8        | 0.16          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 8        | 0.16          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 17       | 0.16          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 17       | 0.16          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 17       | 0.16          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 25       | 0.16          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 25       | 0.16          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 25       | 0.16          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 38       | 0.16          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 38       | 0.16          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 38       | 0.16          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 10       | 0.16          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 10       | 0.16          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 10       | 0.16          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 14       | 0.16          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 14       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 14       | 0.16          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 26       | 0.16          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 26       | 0.16          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 26       | 0.16          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 36       | 0.16          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 36       | 0.16          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 36       | 0.16          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 37       | 0.16          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 37       | 0.16          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 37       | 0.16          |
| (3,1243) | 1:13:A:THR:HG21 | 1:34:A:SER:H    | 34       | 0.16          |
| (3,1243) | 1:13:A:THR:HG22 | 1:34:A:SER:H    | 34       | 0.16          |
| (3,1243) | 1:13:A:THR:HG23 | 1:34:A:SER:H    | 34       | 0.16          |
| (3,1240) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3  | 17       | 0.16          |
| (3,1240) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3  | 17       | 0.16          |
| (3,1240) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3  | 17       | 0.16          |
| (3,1221) | 1:69:A:HIS:H    | 1:56:A:ASN:H    | 19       | 0.16          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 2        | 0.16          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 2        | 0.16          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 2        | 0.16          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 11       | 0.16          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 11       | 0.16          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 11       | 0.16          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 36       | 0.16          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 36       | 0.16          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 36       | 0.16          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 3        | 0.16          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 3        | 0.16          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 3        | 0.16          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 21       | 0.16          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 21       | 0.16          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 21       | 0.16          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 29       | 0.16          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 29       | 0.16          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 29       | 0.16          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 31       | 0.16          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 31       | 0.16          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 31       | 0.16          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 32       | 0.16          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 32       | 0.16          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 32       | 0.16          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 38       | 0.16          |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (3,1194) | 1:22:A:SER:H  | 1:21:A:VAL:HG22 | 38       | 0.16          |
| (3,1194) | 1:22:A:SER:H  | 1:21:A:VAL:HG23 | 38       | 0.16          |
| (3,1189) | 1:21:A:VAL:H  | 1:100:A:GLU:HB3 | 4        | 0.16          |
| (3,1181) | 1:100:A:GLU:H | 1:21:A:VAL:HG11 | 9        | 0.16          |
| (3,1181) | 1:100:A:GLU:H | 1:21:A:VAL:HG12 | 9        | 0.16          |
| (3,1181) | 1:100:A:GLU:H | 1:21:A:VAL:HG13 | 9        | 0.16          |
| (3,1180) | 1:47:A:THR:H  | 1:44:A:LYS:HB3  | 19       | 0.16          |
| (3,1178) | 1:91:A:ALA:H  | 1:84:A:ARG:HA   | 1        | 0.16          |
| (3,1178) | 1:91:A:ALA:H  | 1:84:A:ARG:HA   | 17       | 0.16          |
| (3,1178) | 1:91:A:ALA:H  | 1:84:A:ARG:HA   | 18       | 0.16          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 1        | 0.16          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 1        | 0.16          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 2        | 0.16          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 2        | 0.16          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 20       | 0.16          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 20       | 0.16          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 27       | 0.16          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 27       | 0.16          |
| (3,1152) | 1:54:A:LYS:H  | 1:53:A:GLN:HG3  | 22       | 0.16          |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 4        | 0.16          |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 40       | 0.16          |
| (3,1126) | 1:78:A:VAL:H  | 1:44:A:LYS:HE2  | 20       | 0.16          |
| (3,1096) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 5        | 0.16          |
| (3,1019) | 1:48:A:GLU:H  | 1:48:A:GLU:HG3  | 12       | 0.16          |
| (3,1019) | 1:48:A:GLU:H  | 1:48:A:GLU:HG3  | 15       | 0.16          |
| (3,1019) | 1:48:A:GLU:H  | 1:48:A:GLU:HG3  | 39       | 0.16          |
| (3,988)  | 1:12:A:PHE:H  | 1:11:A:GLN:HB2  | 1        | 0.16          |
| (3,968)  | 1:21:A:VAL:H  | 1:99:A:GLY:HA3  | 6        | 0.16          |
| (3,968)  | 1:21:A:VAL:H  | 1:99:A:GLY:HA3  | 9        | 0.16          |
| (3,968)  | 1:21:A:VAL:H  | 1:99:A:GLY:HA3  | 11       | 0.16          |
| (3,942)  | 1:34:A:SER:H  | 1:12:A:PHE:HA   | 34       | 0.16          |
| (3,934)  | 1:98:A:LYS:H  | 1:20:A:VAL:HG11 | 19       | 0.16          |
| (3,934)  | 1:98:A:LYS:H  | 1:20:A:VAL:HG12 | 19       | 0.16          |
| (3,934)  | 1:98:A:LYS:H  | 1:20:A:VAL:HG13 | 19       | 0.16          |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 2        | 0.16          |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 11       | 0.16          |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 20       | 0.16          |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 25       | 0.16          |
| (3,933)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 27       | 0.16          |
| (3,920)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB2  | 31       | 0.16          |
| (3,889)  | 1:80:A:SER:H  | 1:43:A:TYR:HB3  | 2        | 0.16          |
| (3,889)  | 1:80:A:SER:H  | 1:43:A:TYR:HB3  | 17       | 0.16          |

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| Key     | Atom-1       | Atom-2         | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (3,889) | 1:80:A:SER:H | 1:43:A:TYR:HB3 | 22       | 0.16          |
| (3,889) | 1:80:A:SER:H | 1:43:A:TYR:HB3 | 25       | 0.16          |
| (3,889) | 1:80:A:SER:H | 1:43:A:TYR:HB3 | 29       | 0.16          |
| (3,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3  | 7        | 0.16          |
| (3,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3  | 10       | 0.16          |
| (3,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3  | 11       | 0.16          |
| (3,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3  | 15       | 0.16          |
| (3,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3  | 20       | 0.16          |
| (3,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3  | 21       | 0.16          |
| (3,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2  | 32       | 0.16          |
| (3,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2  | 33       | 0.16          |
| (3,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2  | 36       | 0.16          |
| (3,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA   | 11       | 0.16          |
| (3,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA   | 12       | 0.16          |
| (3,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA   | 14       | 0.16          |
| (3,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA   | 17       | 0.16          |
| (3,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA   | 23       | 0.16          |
| (3,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA   | 25       | 0.16          |
| (3,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA   | 28       | 0.16          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1 | 5        | 0.16          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2 | 5        | 0.16          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3 | 5        | 0.16          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 1        | 0.16          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 2        | 0.16          |
| (3,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 15       | 0.16          |
| (3,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB  | 10       | 0.16          |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2 | 3        | 0.16          |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2 | 10       | 0.16          |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2 | 24       | 0.16          |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2 | 27       | 0.16          |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2 | 29       | 0.16          |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2 | 33       | 0.16          |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2 | 38       | 0.16          |
| (3,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2 | 40       | 0.16          |
| (3,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 1        | 0.16          |
| (3,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 4        | 0.16          |
| (3,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 6        | 0.16          |
| (3,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 10       | 0.16          |
| (3,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 13       | 0.16          |
| (3,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 15       | 0.16          |
| (3,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 17       | 0.16          |
| (3,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 18       | 0.16          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (3,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 23       | 0.16          |
| (3,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 24       | 0.16          |
| (3,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 29       | 0.16          |
| (3,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 31       | 0.16          |
| (3,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 39       | 0.16          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 4        | 0.16          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 6        | 0.16          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 15       | 0.16          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 29       | 0.16          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 33       | 0.16          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 29       | 0.16          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 34       | 0.16          |
| (3,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 1        | 0.16          |
| (3,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 2        | 0.16          |
| (3,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 5        | 0.16          |
| (3,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 8        | 0.16          |
| (3,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 10       | 0.16          |
| (3,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 12       | 0.16          |
| (3,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 14       | 0.16          |
| (3,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 16       | 0.16          |
| (3,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 29       | 0.16          |
| (3,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 39       | 0.16          |
| (3,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 40       | 0.16          |
| (3,591) | 1:3:A:ASP:H   | 1:3:A:ASP:HA    | 13       | 0.16          |
| (3,591) | 1:3:A:ASP:H   | 1:3:A:ASP:HA    | 34       | 0.16          |
| (3,589) | 1:93:A:SER:H  | 1:92:A:ARG:HG2  | 1        | 0.16          |
| (3,589) | 1:93:A:SER:H  | 1:92:A:ARG:HG2  | 13       | 0.16          |
| (3,589) | 1:93:A:SER:H  | 1:92:A:ARG:HG2  | 22       | 0.16          |
| (3,589) | 1:93:A:SER:H  | 1:92:A:ARG:HG2  | 39       | 0.16          |
| (3,560) | 1:47:A:THR:H  | 1:47:A:THR:HA   | 4        | 0.16          |
| (3,560) | 1:47:A:THR:H  | 1:47:A:THR:HA   | 8        | 0.16          |
| (3,560) | 1:47:A:THR:H  | 1:47:A:THR:HA   | 14       | 0.16          |
| (3,560) | 1:47:A:THR:H  | 1:47:A:THR:HA   | 15       | 0.16          |
| (3,560) | 1:47:A:THR:H  | 1:47:A:THR:HA   | 16       | 0.16          |
| (3,560) | 1:47:A:THR:H  | 1:47:A:THR:HA   | 27       | 0.16          |
| (3,560) | 1:47:A:THR:H  | 1:47:A:THR:HA   | 28       | 0.16          |
| (3,560) | 1:47:A:THR:H  | 1:47:A:THR:HA   | 38       | 0.16          |
| (3,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 2        | 0.16          |
| (3,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2  | 2        | 0.16          |
| (3,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 8        | 0.16          |
| (3,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2  | 8        | 0.16          |
| (3,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 21       | 0.16          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2  | 21       | 0.16          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1  | 22       | 0.16          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2  | 22       | 0.16          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1  | 33       | 0.16          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2  | 33       | 0.16          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1  | 34       | 0.16          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2  | 34       | 0.16          |
| (3,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 15       | 0.16          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 4        | 0.16          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 15       | 0.16          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 16       | 0.16          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 38       | 0.16          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 39       | 0.16          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 40       | 0.16          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 4        | 0.16          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 33       | 0.16          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 35       | 0.16          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 38       | 0.16          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 39       | 0.16          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 1        | 0.16          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 12       | 0.16          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 17       | 0.16          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 28       | 0.16          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 29       | 0.16          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 30       | 0.16          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 18       | 0.16          |
| (3,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 31       | 0.16          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 22       | 0.16          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 31       | 0.16          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 34       | 0.16          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 36       | 0.16          |
| (3,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 9        | 0.16          |
| (3,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 19       | 0.16          |
| (3,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 28       | 0.16          |
| (3,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 31       | 0.16          |
| (3,410) | 1:96:A:GLU:H | 1:18:A:ASN:HD21 | 17       | 0.16          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 8        | 0.16          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 13       | 0.16          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 15       | 0.16          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 22       | 0.16          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 23       | 0.16          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 25       | 0.16          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 26       | 0.16          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 29       | 0.16          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 30       | 0.16          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 35       | 0.16          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 38       | 0.16          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 39       | 0.16          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 22       | 0.16          |
| (3,393) | 1:77:A:GLY:H | 1:96:A:GLU:HA   | 20       | 0.16          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 5        | 0.16          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 5        | 0.16          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 5        | 0.16          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 8        | 0.16          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 8        | 0.16          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 8        | 0.16          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 10       | 0.16          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 10       | 0.16          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 10       | 0.16          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 14       | 0.16          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 14       | 0.16          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 14       | 0.16          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 30       | 0.16          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 30       | 0.16          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 30       | 0.16          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 31       | 0.16          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 31       | 0.16          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 31       | 0.16          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 2        | 0.16          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 2        | 0.16          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 2        | 0.16          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 3        | 0.16          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 3        | 0.16          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 3        | 0.16          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 5        | 0.16          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 5        | 0.16          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 5        | 0.16          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 12       | 0.16          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 12       | 0.16          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 12       | 0.16          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 14       | 0.16          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 14       | 0.16          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 14       | 0.16          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 24       | 0.16          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (3,370) | 1:18:A:ASN:H  | 1:95:A:ALA:HB2  | 24       | 0.16          |
| (3,370) | 1:18:A:ASN:H  | 1:95:A:ALA:HB3  | 24       | 0.16          |
| (3,370) | 1:18:A:ASN:H  | 1:95:A:ALA:HB1  | 25       | 0.16          |
| (3,370) | 1:18:A:ASN:H  | 1:95:A:ALA:HB2  | 25       | 0.16          |
| (3,370) | 1:18:A:ASN:H  | 1:95:A:ALA:HB3  | 25       | 0.16          |
| (3,370) | 1:18:A:ASN:H  | 1:95:A:ALA:HB1  | 30       | 0.16          |
| (3,370) | 1:18:A:ASN:H  | 1:95:A:ALA:HB2  | 30       | 0.16          |
| (3,370) | 1:18:A:ASN:H  | 1:95:A:ALA:HB3  | 30       | 0.16          |
| (3,370) | 1:18:A:ASN:H  | 1:95:A:ALA:HB1  | 32       | 0.16          |
| (3,370) | 1:18:A:ASN:H  | 1:95:A:ALA:HB2  | 32       | 0.16          |
| (3,370) | 1:18:A:ASN:H  | 1:95:A:ALA:HB3  | 32       | 0.16          |
| (3,368) | 1:18:A:ASN:H  | 1:17:A:GLN:HB3  | 29       | 0.16          |
| (3,343) | 1:14:A:LYS:H  | 1:33:A:VAL:HA   | 9        | 0.16          |
| (3,343) | 1:14:A:LYS:H  | 1:33:A:VAL:HA   | 13       | 0.16          |
| (3,314) | 1:63:A:CYS:H  | 1:64:A:HIS:HD2  | 31       | 0.16          |
| (3,296) | 1:31:A:CYS:H  | 1:30:A:GLU:HB3  | 1        | 0.16          |
| (3,296) | 1:31:A:CYS:H  | 1:30:A:GLU:HB3  | 11       | 0.16          |
| (3,296) | 1:31:A:CYS:H  | 1:30:A:GLU:HB3  | 22       | 0.16          |
| (3,296) | 1:31:A:CYS:H  | 1:30:A:GLU:HB3  | 25       | 0.16          |
| (3,296) | 1:31:A:CYS:H  | 1:30:A:GLU:HB3  | 30       | 0.16          |
| (3,296) | 1:31:A:CYS:H  | 1:30:A:GLU:HB3  | 36       | 0.16          |
| (3,296) | 1:31:A:CYS:H  | 1:30:A:GLU:HB3  | 37       | 0.16          |
| (3,274) | 1:66:A:MET:H  | 1:66:A:MET:HG3  | 10       | 0.16          |
| (3,274) | 1:66:A:MET:H  | 1:66:A:MET:HG3  | 16       | 0.16          |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 1        | 0.16          |
| (3,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 9        | 0.16          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD1  | 12       | 0.16          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD2  | 12       | 0.16          |
| (3,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 4        | 0.16          |
| (3,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 16       | 0.16          |
| (3,198) | 1:90:A:GLU:H  | 1:90:A:GLU:HB2  | 21       | 0.16          |
| (3,198) | 1:90:A:GLU:H  | 1:90:A:GLU:HB2  | 24       | 0.16          |
| (3,198) | 1:90:A:GLU:H  | 1:90:A:GLU:HB2  | 25       | 0.16          |
| (3,198) | 1:90:A:GLU:H  | 1:90:A:GLU:HB2  | 32       | 0.16          |
| (3,198) | 1:90:A:GLU:H  | 1:90:A:GLU:HB2  | 35       | 0.16          |
| (3,198) | 1:90:A:GLU:H  | 1:90:A:GLU:HB2  | 40       | 0.16          |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 4        | 0.16          |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 40       | 0.16          |
| (3,135) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 7        | 0.16          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 1        | 0.16          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 5        | 0.16          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 8        | 0.16          |

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| Key    | Atom-1       | Atom-2         | Model ID | Violation (Å) |
|--------|--------------|----------------|----------|---------------|
| (3,72) | 1:51:A:GLU:H | 1:51:A:GLU:HG2 | 10       | 0.16          |
| (3,72) | 1:51:A:GLU:H | 1:51:A:GLU:HG2 | 13       | 0.16          |
| (3,72) | 1:51:A:GLU:H | 1:51:A:GLU:HG2 | 16       | 0.16          |
| (3,72) | 1:51:A:GLU:H | 1:51:A:GLU:HG2 | 20       | 0.16          |
| (3,72) | 1:51:A:GLU:H | 1:51:A:GLU:HG2 | 37       | 0.16          |
| (3,59) | 1:42:A:TRP:H | 1:41:A:THR:HB  | 10       | 0.16          |
| (3,59) | 1:42:A:TRP:H | 1:41:A:THR:HB  | 11       | 0.16          |
| (3,59) | 1:42:A:TRP:H | 1:41:A:THR:HB  | 12       | 0.16          |
| (3,59) | 1:42:A:TRP:H | 1:41:A:THR:HB  | 13       | 0.16          |
| (3,59) | 1:42:A:TRP:H | 1:41:A:THR:HB  | 14       | 0.16          |
| (3,59) | 1:42:A:TRP:H | 1:41:A:THR:HB  | 20       | 0.16          |
| (3,59) | 1:42:A:TRP:H | 1:41:A:THR:HB  | 21       | 0.16          |
| (3,59) | 1:42:A:TRP:H | 1:41:A:THR:HB  | 23       | 0.16          |
| (3,59) | 1:42:A:TRP:H | 1:41:A:THR:HB  | 24       | 0.16          |
| (3,59) | 1:42:A:TRP:H | 1:41:A:THR:HB  | 35       | 0.16          |
| (3,59) | 1:42:A:TRP:H | 1:41:A:THR:HB  | 36       | 0.16          |
| (3,51) | 1:57:A:PHE:H | 1:56:A:ASN:HB2 | 7        | 0.16          |
| (3,51) | 1:57:A:PHE:H | 1:56:A:ASN:HB2 | 14       | 0.16          |
| (3,51) | 1:57:A:PHE:H | 1:56:A:ASN:HB2 | 17       | 0.16          |
| (3,51) | 1:57:A:PHE:H | 1:56:A:ASN:HB2 | 25       | 0.16          |
| (3,25) | 1:89:A:GLY:H | 1:88:A:ARG:HB3 | 4        | 0.16          |
| (3,25) | 1:89:A:GLY:H | 1:88:A:ARG:HB3 | 5        | 0.16          |
| (3,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 1        | 0.16          |
| (3,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 2        | 0.16          |
| (3,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 3        | 0.16          |
| (3,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 4        | 0.16          |
| (3,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 5        | 0.16          |
| (3,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 7        | 0.16          |
| (3,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 8        | 0.16          |
| (3,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 9        | 0.16          |
| (3,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 10       | 0.16          |
| (3,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 12       | 0.16          |
| (3,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 13       | 0.16          |
| (3,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 14       | 0.16          |
| (3,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 16       | 0.16          |
| (3,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 17       | 0.16          |
| (3,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 20       | 0.16          |
| (3,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 21       | 0.16          |
| (3,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 22       | 0.16          |
| (3,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 23       | 0.16          |
| (3,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 24       | 0.16          |
| (3,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 25       | 0.16          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 26       | 0.16          |
| (3,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 27       | 0.16          |
| (3,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 28       | 0.16          |
| (3,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 30       | 0.16          |
| (3,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 32       | 0.16          |
| (3,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 34       | 0.16          |
| (3,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 35       | 0.16          |
| (3,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 37       | 0.16          |
| (3,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 38       | 0.16          |
| (3,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 39       | 0.16          |
| (3,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 40       | 0.16          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 3        | 0.16          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 3        | 0.16          |
| (1,3211) | 1:69:A:HIS:HE1 | 1:67:A:THR:HB   | 23       | 0.16          |
| (1,3211) | 1:69:A:HIS:HE1 | 1:67:A:THR:HB   | 25       | 0.16          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 8        | 0.16          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 8        | 0.16          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 14       | 0.16          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 14       | 0.16          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 39       | 0.16          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 39       | 0.16          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 6        | 0.16          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 6        | 0.16          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 6        | 0.16          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 6        | 0.16          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 6        | 0.16          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 6        | 0.16          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 35       | 0.16          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 35       | 0.16          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 35       | 0.16          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 35       | 0.16          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 35       | 0.16          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 35       | 0.16          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 39       | 0.16          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 39       | 0.16          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 39       | 0.16          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 39       | 0.16          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 39       | 0.16          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 39       | 0.16          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 4        | 0.16          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 4        | 0.16          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 4        | 0.16          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2 | 4        | 0.16          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1 | 19       | 0.16          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2 | 19       | 0.16          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1 | 19       | 0.16          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2 | 19       | 0.16          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1 | 24       | 0.16          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2 | 24       | 0.16          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1 | 24       | 0.16          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2 | 24       | 0.16          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1 | 29       | 0.16          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2 | 29       | 0.16          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1 | 29       | 0.16          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2 | 29       | 0.16          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB  | 19       | 0.16          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB  | 24       | 0.16          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB  | 35       | 0.16          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB  | 38       | 0.16          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB  | 39       | 0.16          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1 | 29       | 0.16          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2 | 29       | 0.16          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3 | 29       | 0.16          |
| (1,3158) | 1:42:A:TRP:HD1 | 1:41:A:THR:HA  | 16       | 0.16          |
| (1,3137) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3 | 25       | 0.16          |
| (1,3137) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3 | 25       | 0.16          |
| (1,3137) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3 | 30       | 0.16          |
| (1,3137) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3 | 30       | 0.16          |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 4        | 0.16          |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 4        | 0.16          |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 18       | 0.16          |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 18       | 0.16          |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 25       | 0.16          |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 25       | 0.16          |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 32       | 0.16          |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 32       | 0.16          |
| (1,3131) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3 | 14       | 0.16          |
| (1,3131) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3 | 14       | 0.16          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 2        | 0.16          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 2        | 0.16          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 8        | 0.16          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 8        | 0.16          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 16       | 0.16          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 16       | 0.16          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 23       | 0.16          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 23       | 0.16          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 32       | 0.16          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 32       | 0.16          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 38       | 0.16          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 38       | 0.16          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 39       | 0.16          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 39       | 0.16          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 2        | 0.16          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 2        | 0.16          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 8        | 0.16          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 8        | 0.16          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 16       | 0.16          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 16       | 0.16          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 23       | 0.16          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 23       | 0.16          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 32       | 0.16          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 32       | 0.16          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 38       | 0.16          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 38       | 0.16          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 39       | 0.16          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 39       | 0.16          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 9        | 0.16          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 9        | 0.16          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 9        | 0.16          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 9        | 0.16          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 9        | 0.16          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 9        | 0.16          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 13       | 0.16          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 13       | 0.16          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 13       | 0.16          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 13       | 0.16          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 13       | 0.16          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 13       | 0.16          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 17       | 0.16          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 17       | 0.16          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 17       | 0.16          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 17       | 0.16          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 17       | 0.16          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 17       | 0.16          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 26       | 0.16          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 26       | 0.16          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 26       | 0.16          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 26       | 0.16          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 26       | 0.16          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 26       | 0.16          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 35       | 0.16          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 35       | 0.16          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 35       | 0.16          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 35       | 0.16          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 35       | 0.16          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 35       | 0.16          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 2        | 0.16          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 2        | 0.16          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 2        | 0.16          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 2        | 0.16          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 2        | 0.16          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 2        | 0.16          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 8        | 0.16          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 8        | 0.16          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 8        | 0.16          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 8        | 0.16          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 8        | 0.16          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 8        | 0.16          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 9        | 0.16          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 9        | 0.16          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 9        | 0.16          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 9        | 0.16          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 9        | 0.16          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 9        | 0.16          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 13       | 0.16          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 13       | 0.16          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 13       | 0.16          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 13       | 0.16          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 13       | 0.16          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 13       | 0.16          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 18       | 0.16          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 18       | 0.16          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 18       | 0.16          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 18       | 0.16          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 18       | 0.16          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 18       | 0.16          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 32       | 0.16          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 32       | 0.16          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 32       | 0.16          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 32       | 0.16          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 19       | 0.16          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 19       | 0.16          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 19       | 0.16          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 19       | 0.16          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 19       | 0.16          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 19       | 0.16          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 29       | 0.16          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 29       | 0.16          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 29       | 0.16          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 29       | 0.16          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 29       | 0.16          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 29       | 0.16          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 9        | 0.16          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 10       | 0.16          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 13       | 0.16          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 21       | 0.16          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 22       | 0.16          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 23       | 0.16          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 24       | 0.16          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 25       | 0.16          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 26       | 0.16          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 27       | 0.16          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 28       | 0.16          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 30       | 0.16          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 31       | 0.16          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 32       | 0.16          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 35       | 0.16          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 36       | 0.16          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 38       | 0.16          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 39       | 0.16          |
| (1,3088) | 1:88:A:ARG:HD2 | 1:88:A:ARG:HA   | 40       | 0.16          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 8        | 0.16          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 8        | 0.16          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 8        | 0.16          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 29       | 0.16          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 29       | 0.16          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 29       | 0.16          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 32       | 0.16          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 32       | 0.16          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 37       | 0.16          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 37       | 0.16          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB2  | 31       | 0.16          |
| (1,3069) | 1:87:A:PRO:HD2 | 1:86:A:GLU:HB3  | 31       | 0.16          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 3        | 0.16          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 18       | 0.16          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 22       | 0.16          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 2        | 0.16          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 2        | 0.16          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 3        | 0.16          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 3        | 0.16          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 1        | 0.16          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 1        | 0.16          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 1        | 0.16          |
| (1,3011) | 1:30:A:GLU:HB2 | 1:14:A:LYS:HE2  | 14       | 0.16          |
| (1,3011) | 1:30:A:GLU:HB2 | 1:14:A:LYS:HE2  | 35       | 0.16          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 14       | 0.16          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 14       | 0.16          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 14       | 0.16          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 29       | 0.16          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 29       | 0.16          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 29       | 0.16          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 30       | 0.16          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 30       | 0.16          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 30       | 0.16          |
| (1,2996) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 14       | 0.16          |
| (1,2996) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 24       | 0.16          |
| (1,2962) | 1:44:A:LYS:HE2 | 1:44:A:LYS:HG3  | 20       | 0.16          |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1  | 25       | 0.16          |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2  | 25       | 0.16          |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1  | 30       | 0.16          |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2  | 30       | 0.16          |
| (1,2931) | 1:26:A:SER:HA  | 1:70:A:ASN:H    | 15       | 0.16          |
| (1,2931) | 1:26:A:SER:HA  | 1:70:A:ASN:H    | 29       | 0.16          |
| (1,2903) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD2  | 13       | 0.16          |
| (1,2903) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD2  | 20       | 0.16          |
| (1,2903) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD2  | 27       | 0.16          |
| (1,2903) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD2  | 28       | 0.16          |
| (1,2903) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD2  | 29       | 0.16          |
| (1,2859) | 1:92:A:ARG:HB3 | 1:92:A:ARG:H    | 1        | 0.16          |
| (1,2859) | 1:92:A:ARG:HB3 | 1:92:A:ARG:H    | 3        | 0.16          |
| (1,2859) | 1:92:A:ARG:HB3 | 1:92:A:ARG:H    | 5        | 0.16          |
| (1,2859) | 1:92:A:ARG:HB3 | 1:92:A:ARG:H    | 7        | 0.16          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (1,2859) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H  | 8        | 0.16          |
| (1,2859) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H  | 15       | 0.16          |
| (1,2859) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H  | 16       | 0.16          |
| (1,2859) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H  | 26       | 0.16          |
| (1,2859) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H  | 29       | 0.16          |
| (1,2859) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H  | 36       | 0.16          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H | 4        | 0.16          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H | 6        | 0.16          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H | 15       | 0.16          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H | 29       | 0.16          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H | 33       | 0.16          |
| (1,2754) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H  | 1        | 0.16          |
| (1,2754) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H  | 5        | 0.16          |
| (1,2754) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H  | 9        | 0.16          |
| (1,2754) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H  | 10       | 0.16          |
| (1,2754) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H  | 33       | 0.16          |
| (1,2754) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H  | 37       | 0.16          |
| (1,2745) | 1:86:A:GLU:HG2  | 1:86:A:GLU:H  | 17       | 0.16          |
| (1,2745) | 1:86:A:GLU:HG3  | 1:86:A:GLU:H  | 17       | 0.16          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 8        | 0.16          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 13       | 0.16          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 15       | 0.16          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 22       | 0.16          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 23       | 0.16          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 25       | 0.16          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 26       | 0.16          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 29       | 0.16          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 30       | 0.16          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 35       | 0.16          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 38       | 0.16          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 39       | 0.16          |
| (1,2686) | 1:8:A:GLU:HB3   | 1:8:A:GLU:HG2 | 4        | 0.16          |
| (1,2686) | 1:8:A:GLU:HB3   | 1:8:A:GLU:HG2 | 5        | 0.16          |
| (1,2686) | 1:8:A:GLU:HB3   | 1:8:A:GLU:HG2 | 18       | 0.16          |
| (1,2686) | 1:8:A:GLU:HB3   | 1:8:A:GLU:HG2 | 19       | 0.16          |
| (1,2686) | 1:8:A:GLU:HB3   | 1:8:A:GLU:HG2 | 27       | 0.16          |
| (1,2675) | 1:25:A:GLN:HG3  | 1:26:A:SER:H  | 4        | 0.16          |
| (1,2675) | 1:25:A:GLN:HG3  | 1:26:A:SER:H  | 10       | 0.16          |
| (1,2675) | 1:25:A:GLN:HG3  | 1:26:A:SER:H  | 11       | 0.16          |
| (1,2675) | 1:25:A:GLN:HG3  | 1:26:A:SER:H  | 12       | 0.16          |
| (1,2675) | 1:25:A:GLN:HG3  | 1:26:A:SER:H  | 28       | 0.16          |
| (1,2675) | 1:25:A:GLN:HG3  | 1:26:A:SER:H  | 30       | 0.16          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 6        | 0.16          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 6        | 0.16          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 6        | 0.16          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 7        | 0.16          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 7        | 0.16          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 7        | 0.16          |
| (1,2598) | 1:36:A:ASP:HB2 | 1:37:A:ASP:H    | 31       | 0.16          |
| (1,2550) | 1:92:A:ARG:HA  | 1:83:A:ALA:H    | 18       | 0.16          |
| (1,2550) | 1:92:A:ARG:HA  | 1:83:A:ALA:H    | 28       | 0.16          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA   | 16       | 0.16          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA    | 11       | 0.16          |
| (1,2485) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3   | 3        | 0.16          |
| (1,2485) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3   | 4        | 0.16          |
| (1,2485) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3   | 8        | 0.16          |
| (1,2485) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3   | 14       | 0.16          |
| (1,2485) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3   | 16       | 0.16          |
| (1,2485) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3   | 17       | 0.16          |
| (1,2475) | 1:4:A:PRO:HG3  | 1:4:A:PRO:HG2   | 1        | 0.16          |
| (1,2475) | 1:4:A:PRO:HG3  | 1:4:A:PRO:HG2   | 4        | 0.16          |
| (1,2475) | 1:4:A:PRO:HG3  | 1:4:A:PRO:HG2   | 9        | 0.16          |
| (1,2475) | 1:4:A:PRO:HG3  | 1:4:A:PRO:HG2   | 10       | 0.16          |
| (1,2475) | 1:4:A:PRO:HG3  | 1:4:A:PRO:HG2   | 12       | 0.16          |
| (1,2475) | 1:4:A:PRO:HG3  | 1:4:A:PRO:HG2   | 15       | 0.16          |
| (1,2475) | 1:4:A:PRO:HG3  | 1:4:A:PRO:HG2   | 16       | 0.16          |
| (1,2475) | 1:4:A:PRO:HG3  | 1:4:A:PRO:HG2   | 17       | 0.16          |
| (1,2475) | 1:4:A:PRO:HG3  | 1:4:A:PRO:HG2   | 18       | 0.16          |
| (1,2475) | 1:4:A:PRO:HG3  | 1:4:A:PRO:HG2   | 35       | 0.16          |
| (1,2474) | 1:4:A:PRO:HG2  | 1:4:A:PRO:HG3   | 1        | 0.16          |
| (1,2474) | 1:4:A:PRO:HG2  | 1:4:A:PRO:HG3   | 4        | 0.16          |
| (1,2474) | 1:4:A:PRO:HG2  | 1:4:A:PRO:HG3   | 9        | 0.16          |
| (1,2474) | 1:4:A:PRO:HG2  | 1:4:A:PRO:HG3   | 10       | 0.16          |
| (1,2474) | 1:4:A:PRO:HG2  | 1:4:A:PRO:HG3   | 12       | 0.16          |
| (1,2474) | 1:4:A:PRO:HG2  | 1:4:A:PRO:HG3   | 15       | 0.16          |
| (1,2474) | 1:4:A:PRO:HG2  | 1:4:A:PRO:HG3   | 16       | 0.16          |
| (1,2474) | 1:4:A:PRO:HG2  | 1:4:A:PRO:HG3   | 17       | 0.16          |
| (1,2474) | 1:4:A:PRO:HG2  | 1:4:A:PRO:HG3   | 18       | 0.16          |
| (1,2474) | 1:4:A:PRO:HG2  | 1:4:A:PRO:HG3   | 35       | 0.16          |
| (1,2460) | 1:4:A:PRO:HD3  | 1:3:A:ASP:HA    | 3        | 0.16          |
| (1,2431) | 1:82:A:ILE:HB  | 1:41:A:THR:H    | 19       | 0.16          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2  | 13       | 0.16          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2  | 31       | 0.16          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2  | 33       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2409) | 1:10:A:ILE:HA   | 1:11:A:GLN:HG2  | 35       | 0.16          |
| (1,2409) | 1:10:A:ILE:HA   | 1:11:A:GLN:HG2  | 36       | 0.16          |
| (1,2403) | 1:66:A:MET:HE1  | 1:42:A:TRP:H    | 9        | 0.16          |
| (1,2403) | 1:66:A:MET:HE2  | 1:42:A:TRP:H    | 9        | 0.16          |
| (1,2403) | 1:66:A:MET:HE3  | 1:42:A:TRP:H    | 9        | 0.16          |
| (1,2403) | 1:66:A:MET:HE1  | 1:42:A:TRP:H    | 13       | 0.16          |
| (1,2403) | 1:66:A:MET:HE2  | 1:42:A:TRP:H    | 13       | 0.16          |
| (1,2403) | 1:66:A:MET:HE3  | 1:42:A:TRP:H    | 13       | 0.16          |
| (1,2403) | 1:66:A:MET:HE1  | 1:42:A:TRP:H    | 14       | 0.16          |
| (1,2403) | 1:66:A:MET:HE2  | 1:42:A:TRP:H    | 14       | 0.16          |
| (1,2403) | 1:66:A:MET:HE3  | 1:42:A:TRP:H    | 14       | 0.16          |
| (1,2403) | 1:66:A:MET:HE1  | 1:42:A:TRP:H    | 18       | 0.16          |
| (1,2403) | 1:66:A:MET:HE2  | 1:42:A:TRP:H    | 18       | 0.16          |
| (1,2403) | 1:66:A:MET:HE3  | 1:42:A:TRP:H    | 18       | 0.16          |
| (1,2403) | 1:66:A:MET:HE1  | 1:42:A:TRP:H    | 27       | 0.16          |
| (1,2403) | 1:66:A:MET:HE2  | 1:42:A:TRP:H    | 27       | 0.16          |
| (1,2403) | 1:66:A:MET:HE3  | 1:42:A:TRP:H    | 27       | 0.16          |
| (1,2403) | 1:66:A:MET:HE1  | 1:42:A:TRP:H    | 32       | 0.16          |
| (1,2403) | 1:66:A:MET:HE2  | 1:42:A:TRP:H    | 32       | 0.16          |
| (1,2403) | 1:66:A:MET:HE3  | 1:42:A:TRP:H    | 32       | 0.16          |
| (1,2402) | 1:66:A:MET:HE1  | 1:29:A:PHE:HZ   | 15       | 0.16          |
| (1,2402) | 1:66:A:MET:HE2  | 1:29:A:PHE:HZ   | 15       | 0.16          |
| (1,2402) | 1:66:A:MET:HE3  | 1:29:A:PHE:HZ   | 15       | 0.16          |
| (1,2402) | 1:66:A:MET:HE1  | 1:29:A:PHE:HZ   | 35       | 0.16          |
| (1,2402) | 1:66:A:MET:HE2  | 1:29:A:PHE:HZ   | 35       | 0.16          |
| (1,2402) | 1:66:A:MET:HE3  | 1:29:A:PHE:HZ   | 35       | 0.16          |
| (1,2287) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 5        | 0.16          |
| (1,2287) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 13       | 0.16          |
| (1,2287) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 16       | 0.16          |
| (1,2287) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 38       | 0.16          |
| (1,2286) | 1:96:A:GLU:HG2  | 1:97:A:LEU:H    | 3        | 0.16          |
| (1,2286) | 1:96:A:GLU:HG2  | 1:97:A:LEU:H    | 5        | 0.16          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 14       | 0.16          |
| (1,2250) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 14       | 0.16          |
| (1,2215) | 1:56:A:ASN:HA   | 1:56:A:ASN:HD21 | 7        | 0.16          |
| (1,2170) | 1:43:A:TYR:HA   | 1:80:A:SER:H    | 8        | 0.16          |
| (1,2145) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 21       | 0.16          |
| (1,2099) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HA   | 24       | 0.16          |
| (1,2099) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HA   | 24       | 0.16          |
| (1,2099) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HA   | 24       | 0.16          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 5        | 0.16          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 5        | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 5        | 0.16          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 27       | 0.16          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 27       | 0.16          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 27       | 0.16          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 37       | 0.16          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 37       | 0.16          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 37       | 0.16          |
| (1,2087) | 1:85:A:LEU:HD11 | 1:39:A:ILE:H    | 4        | 0.16          |
| (1,2087) | 1:85:A:LEU:HD12 | 1:39:A:ILE:H    | 4        | 0.16          |
| (1,2087) | 1:85:A:LEU:HD13 | 1:39:A:ILE:H    | 4        | 0.16          |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD11 | 8        | 0.16          |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD12 | 8        | 0.16          |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD13 | 8        | 0.16          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD11 | 8        | 0.16          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD12 | 8        | 0.16          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD13 | 8        | 0.16          |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD11 | 8        | 0.16          |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD12 | 8        | 0.16          |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD13 | 8        | 0.16          |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD11 | 13       | 0.16          |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD12 | 13       | 0.16          |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD13 | 13       | 0.16          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD11 | 13       | 0.16          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD12 | 13       | 0.16          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD13 | 13       | 0.16          |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD11 | 13       | 0.16          |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD12 | 13       | 0.16          |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD13 | 13       | 0.16          |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD11 | 18       | 0.16          |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD12 | 18       | 0.16          |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD13 | 18       | 0.16          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD11 | 18       | 0.16          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD12 | 18       | 0.16          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD13 | 18       | 0.16          |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD11 | 18       | 0.16          |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD12 | 18       | 0.16          |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD13 | 18       | 0.16          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3  | 12       | 0.16          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3  | 12       | 0.16          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3  | 12       | 0.16          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3  | 15       | 0.16          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3  | 15       | 0.16          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 15       | 0.16          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3 | 17       | 0.16          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3 | 17       | 0.16          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3 | 17       | 0.16          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 15       | 0.16          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 15       | 0.16          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 15       | 0.16          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 15       | 0.16          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 15       | 0.16          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 15       | 0.16          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 9        | 0.16          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 9        | 0.16          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 9        | 0.16          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 26       | 0.16          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 26       | 0.16          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 26       | 0.16          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 32       | 0.16          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 32       | 0.16          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 32       | 0.16          |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 14       | 0.16          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 14       | 0.16          |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 14       | 0.16          |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 29       | 0.16          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 29       | 0.16          |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 29       | 0.16          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 20       | 0.16          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 20       | 0.16          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 20       | 0.16          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 20       | 0.16          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 20       | 0.16          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 20       | 0.16          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 35       | 0.16          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 35       | 0.16          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 35       | 0.16          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 35       | 0.16          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 35       | 0.16          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 35       | 0.16          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 1        | 0.16          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 11       | 0.16          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 22       | 0.16          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 25       | 0.16          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 30       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 36       | 0.16          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 37       | 0.16          |
| (1,2005) | 1:28:A:THR:HG21 | 1:30:A:GLU:HG3  | 19       | 0.16          |
| (1,2005) | 1:28:A:THR:HG22 | 1:30:A:GLU:HG3  | 19       | 0.16          |
| (1,2005) | 1:28:A:THR:HG23 | 1:30:A:GLU:HG3  | 19       | 0.16          |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 11       | 0.16          |
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 11       | 0.16          |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 11       | 0.16          |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 16       | 0.16          |
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 16       | 0.16          |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 16       | 0.16          |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 35       | 0.16          |
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 35       | 0.16          |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 35       | 0.16          |
| (1,1990) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 20       | 0.16          |
| (1,1990) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 20       | 0.16          |
| (1,1990) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 20       | 0.16          |
| (1,1966) | 1:36:A:ASP:HB3  | 1:62:A:ARG:HA   | 7        | 0.16          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 6        | 0.16          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 10       | 0.16          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 24       | 0.16          |
| (1,1952) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB1  | 5        | 0.16          |
| (1,1952) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB2  | 5        | 0.16          |
| (1,1952) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB3  | 5        | 0.16          |
| (1,1952) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB1  | 5        | 0.16          |
| (1,1952) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB2  | 5        | 0.16          |
| (1,1952) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB3  | 5        | 0.16          |
| (1,1952) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB1  | 5        | 0.16          |
| (1,1952) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB2  | 5        | 0.16          |
| (1,1952) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB3  | 5        | 0.16          |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA   | 1        | 0.16          |
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA   | 1        | 0.16          |
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA   | 1        | 0.16          |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA   | 25       | 0.16          |
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA   | 25       | 0.16          |
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA   | 25       | 0.16          |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA   | 34       | 0.16          |
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA   | 34       | 0.16          |
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA   | 34       | 0.16          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H    | 1        | 0.16          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H    | 1        | 0.16          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H    | 1        | 0.16          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 2        | 0.16          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 2        | 0.16          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 2        | 0.16          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 3        | 0.16          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 3        | 0.16          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 3        | 0.16          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 4        | 0.16          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 4        | 0.16          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 4        | 0.16          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 7        | 0.16          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 7        | 0.16          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 7        | 0.16          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 9        | 0.16          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 9        | 0.16          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 9        | 0.16          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 11       | 0.16          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 11       | 0.16          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 11       | 0.16          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 16       | 0.16          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 16       | 0.16          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 16       | 0.16          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 19       | 0.16          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 19       | 0.16          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 19       | 0.16          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 24       | 0.16          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 24       | 0.16          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 24       | 0.16          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 27       | 0.16          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 27       | 0.16          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 27       | 0.16          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 35       | 0.16          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 35       | 0.16          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 35       | 0.16          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 36       | 0.16          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 36       | 0.16          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 36       | 0.16          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 38       | 0.16          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 38       | 0.16          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 38       | 0.16          |
| (1,1861) | 1:7:A:ALA:HB1   | 1:88:A:ARG:HA | 8        | 0.16          |
| (1,1861) | 1:7:A:ALA:HB2   | 1:88:A:ARG:HA | 8        | 0.16          |
| (1,1861) | 1:7:A:ALA:HB3   | 1:88:A:ARG:HA | 8        | 0.16          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1861) | 1:7:A:ALA:HB1  | 1:88:A:ARG:HA  | 32       | 0.16          |
| (1,1861) | 1:7:A:ALA:HB2  | 1:88:A:ARG:HA  | 32       | 0.16          |
| (1,1861) | 1:7:A:ALA:HB3  | 1:88:A:ARG:HA  | 32       | 0.16          |
| (1,1853) | 1:27:A:ALA:HB1 | 1:28:A:THR:H   | 2        | 0.16          |
| (1,1853) | 1:27:A:ALA:HB2 | 1:28:A:THR:H   | 2        | 0.16          |
| (1,1853) | 1:27:A:ALA:HB3 | 1:28:A:THR:H   | 2        | 0.16          |
| (1,1853) | 1:27:A:ALA:HB1 | 1:28:A:THR:H   | 3        | 0.16          |
| (1,1853) | 1:27:A:ALA:HB2 | 1:28:A:THR:H   | 3        | 0.16          |
| (1,1853) | 1:27:A:ALA:HB3 | 1:28:A:THR:H   | 3        | 0.16          |
| (1,1853) | 1:27:A:ALA:HB1 | 1:28:A:THR:H   | 11       | 0.16          |
| (1,1853) | 1:27:A:ALA:HB2 | 1:28:A:THR:H   | 11       | 0.16          |
| (1,1853) | 1:27:A:ALA:HB3 | 1:28:A:THR:H   | 11       | 0.16          |
| (1,1853) | 1:27:A:ALA:HB1 | 1:28:A:THR:H   | 12       | 0.16          |
| (1,1853) | 1:27:A:ALA:HB2 | 1:28:A:THR:H   | 12       | 0.16          |
| (1,1853) | 1:27:A:ALA:HB3 | 1:28:A:THR:H   | 12       | 0.16          |
| (1,1853) | 1:27:A:ALA:HB1 | 1:28:A:THR:H   | 16       | 0.16          |
| (1,1853) | 1:27:A:ALA:HB2 | 1:28:A:THR:H   | 16       | 0.16          |
| (1,1853) | 1:27:A:ALA:HB3 | 1:28:A:THR:H   | 16       | 0.16          |
| (1,1853) | 1:27:A:ALA:HB1 | 1:28:A:THR:H   | 19       | 0.16          |
| (1,1853) | 1:27:A:ALA:HB2 | 1:28:A:THR:H   | 19       | 0.16          |
| (1,1853) | 1:27:A:ALA:HB3 | 1:28:A:THR:H   | 19       | 0.16          |
| (1,1853) | 1:27:A:ALA:HB1 | 1:28:A:THR:H   | 22       | 0.16          |
| (1,1853) | 1:27:A:ALA:HB2 | 1:28:A:THR:H   | 22       | 0.16          |
| (1,1853) | 1:27:A:ALA:HB3 | 1:28:A:THR:H   | 22       | 0.16          |
| (1,1853) | 1:27:A:ALA:HB1 | 1:28:A:THR:H   | 26       | 0.16          |
| (1,1853) | 1:27:A:ALA:HB2 | 1:28:A:THR:H   | 26       | 0.16          |
| (1,1853) | 1:27:A:ALA:HB3 | 1:28:A:THR:H   | 26       | 0.16          |
| (1,1853) | 1:27:A:ALA:HB1 | 1:28:A:THR:H   | 27       | 0.16          |
| (1,1853) | 1:27:A:ALA:HB2 | 1:28:A:THR:H   | 27       | 0.16          |
| (1,1853) | 1:27:A:ALA:HB3 | 1:28:A:THR:H   | 27       | 0.16          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3 | 4        | 0.16          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3 | 5        | 0.16          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3 | 6        | 0.16          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3 | 7        | 0.16          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3 | 8        | 0.16          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3 | 9        | 0.16          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3 | 10       | 0.16          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3 | 13       | 0.16          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3 | 19       | 0.16          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3 | 21       | 0.16          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3 | 22       | 0.16          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3 | 23       | 0.16          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 25       | 0.16          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 29       | 0.16          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 30       | 0.16          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 31       | 0.16          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 32       | 0.16          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 36       | 0.16          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 38       | 0.16          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 39       | 0.16          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 40       | 0.16          |
| (1,1744) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H    | 1        | 0.16          |
| (1,1744) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H    | 5        | 0.16          |
| (1,1744) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H    | 8        | 0.16          |
| (1,1744) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H    | 10       | 0.16          |
| (1,1744) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H    | 13       | 0.16          |
| (1,1744) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H    | 16       | 0.16          |
| (1,1744) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H    | 20       | 0.16          |
| (1,1744) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H    | 37       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG11 | 14       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG12 | 14       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG13 | 14       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG11 | 14       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG12 | 14       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG13 | 14       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG11 | 14       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG12 | 14       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG13 | 14       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG11 | 21       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG12 | 21       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG13 | 21       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG11 | 21       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG12 | 21       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG13 | 21       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG11 | 21       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG12 | 21       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG13 | 21       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG11 | 38       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG12 | 38       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG13 | 38       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG11 | 38       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG12 | 38       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG13 | 38       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG11 | 38       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 38       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 38       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG11 | 39       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG12 | 39       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG13 | 39       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG11 | 39       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG12 | 39       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 39       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 39       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 39       | 0.16          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 39       | 0.16          |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 15       | 0.16          |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 15       | 0.16          |
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 15       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 2        | 0.16          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 2        | 0.16          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 2        | 0.16          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 2        | 0.16          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 2        | 0.16          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 2        | 0.16          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 2        | 0.16          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 2        | 0.16          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 2        | 0.16          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 5        | 0.16          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 5        | 0.16          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 5        | 0.16          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 5        | 0.16          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 5        | 0.16          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 5        | 0.16          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 5        | 0.16          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 5        | 0.16          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 5        | 0.16          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 10       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 10       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 10       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 10       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 10       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 10       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 10       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 10       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 10       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 13       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 13       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 13       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 13       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 13       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 13       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 13       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 13       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 13       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 28       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 28       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 28       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 28       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 28       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 28       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 28       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 28       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 28       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 29       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 29       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 29       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 29       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 29       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 29       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 29       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 29       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 29       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 30       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 30       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 30       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 30       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 30       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 30       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 30       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 30       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 30       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 35       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 35       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 35       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 35       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 35       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 35       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 35       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 35       | 0.16          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 35       | 0.16          |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 26       | 0.16          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 26       | 0.16          |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 26       | 0.16          |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 33       | 0.16          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 33       | 0.16          |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 33       | 0.16          |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 35       | 0.16          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 35       | 0.16          |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 35       | 0.16          |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 37       | 0.16          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 37       | 0.16          |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 37       | 0.16          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 8        | 0.16          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 8        | 0.16          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 8        | 0.16          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 8        | 0.16          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 8        | 0.16          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 8        | 0.16          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 8        | 0.16          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 8        | 0.16          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 8        | 0.16          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 12       | 0.16          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 12       | 0.16          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 12       | 0.16          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 12       | 0.16          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 12       | 0.16          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 12       | 0.16          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 12       | 0.16          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 12       | 0.16          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 12       | 0.16          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 13       | 0.16          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 13       | 0.16          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 13       | 0.16          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 13       | 0.16          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 13       | 0.16          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 13       | 0.16          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 13       | 0.16          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 13       | 0.16          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 13       | 0.16          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 14       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 14       | 0.16          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 14       | 0.16          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 14       | 0.16          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 14       | 0.16          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 14       | 0.16          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 14       | 0.16          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 14       | 0.16          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 14       | 0.16          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 2        | 0.16          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 2        | 0.16          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 2        | 0.16          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 18       | 0.16          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 18       | 0.16          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 18       | 0.16          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 23       | 0.16          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 23       | 0.16          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 23       | 0.16          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 2        | 0.16          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 2        | 0.16          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 2        | 0.16          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 15       | 0.16          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 15       | 0.16          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 15       | 0.16          |
| (1,1619) | 1:82:A:ILE:HD11 | 1:82:A:ILE:HA   | 32       | 0.16          |
| (1,1619) | 1:82:A:ILE:HD12 | 1:82:A:ILE:HA   | 32       | 0.16          |
| (1,1619) | 1:82:A:ILE:HD13 | 1:82:A:ILE:HA   | 32       | 0.16          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 29       | 0.16          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 29       | 0.16          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 29       | 0.16          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1  | 9        | 0.16          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2  | 9        | 0.16          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1  | 9        | 0.16          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2  | 9        | 0.16          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1  | 9        | 0.16          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2  | 9        | 0.16          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1  | 13       | 0.16          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2  | 13       | 0.16          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1  | 13       | 0.16          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2  | 13       | 0.16          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1  | 13       | 0.16          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2  | 13       | 0.16          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1  | 17       | 0.16          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 17       | 0.16          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 17       | 0.16          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 17       | 0.16          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 17       | 0.16          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 17       | 0.16          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 26       | 0.16          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 26       | 0.16          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 26       | 0.16          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 26       | 0.16          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 26       | 0.16          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 26       | 0.16          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 35       | 0.16          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 35       | 0.16          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 35       | 0.16          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 35       | 0.16          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 35       | 0.16          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 35       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 13       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 13       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 13       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 13       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 13       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 13       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 17       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 17       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 17       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 17       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 17       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 17       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 19       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 19       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 19       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 19       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 19       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 19       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 20       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 20       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 20       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 20       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 20       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 20       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 27       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 27       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 27       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 27       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 27       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 27       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 30       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 30       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 30       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 30       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 30       | 0.16          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 30       | 0.16          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 1        | 0.16          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 1        | 0.16          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 1        | 0.16          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 2        | 0.16          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 2        | 0.16          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 2        | 0.16          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 13       | 0.16          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 13       | 0.16          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 13       | 0.16          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 25       | 0.16          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 25       | 0.16          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 25       | 0.16          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 33       | 0.16          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 33       | 0.16          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 33       | 0.16          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 38       | 0.16          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 38       | 0.16          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 38       | 0.16          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 1        | 0.16          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 1        | 0.16          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 1        | 0.16          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 2        | 0.16          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 2        | 0.16          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 2        | 0.16          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 4        | 0.16          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 4        | 0.16          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 4        | 0.16          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 5        | 0.16          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 5        | 0.16          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 5        | 0.16          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 9        | 0.16          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA  | 9        | 0.16          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA  | 9        | 0.16          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA  | 18       | 0.16          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA  | 18       | 0.16          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA  | 18       | 0.16          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA  | 19       | 0.16          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA  | 19       | 0.16          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA  | 19       | 0.16          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA  | 20       | 0.16          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA  | 20       | 0.16          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA  | 20       | 0.16          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA  | 27       | 0.16          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA  | 27       | 0.16          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA  | 27       | 0.16          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA  | 31       | 0.16          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA  | 31       | 0.16          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA  | 31       | 0.16          |
| (1,1543) | 1:2:A:ILE:HG12  | 1:2:A:ILE:HA   | 8        | 0.16          |
| (1,1543) | 1:2:A:ILE:HG12  | 1:2:A:ILE:HA   | 10       | 0.16          |
| (1,1543) | 1:2:A:ILE:HG12  | 1:2:A:ILE:HA   | 14       | 0.16          |
| (1,1543) | 1:2:A:ILE:HG12  | 1:2:A:ILE:HA   | 17       | 0.16          |
| (1,1543) | 1:2:A:ILE:HG12  | 1:2:A:ILE:HA   | 30       | 0.16          |
| (1,1514) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 13       | 0.16          |
| (1,1514) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 13       | 0.16          |
| (1,1514) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 13       | 0.16          |
| (1,1514) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 19       | 0.16          |
| (1,1514) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 19       | 0.16          |
| (1,1514) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 19       | 0.16          |
| (1,1514) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 36       | 0.16          |
| (1,1514) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 36       | 0.16          |
| (1,1514) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 36       | 0.16          |
| (1,1510) | 1:66:A:MET:HE1  | 1:42:A:TRP:HE1 | 29       | 0.16          |
| (1,1510) | 1:66:A:MET:HE2  | 1:42:A:TRP:HE1 | 29       | 0.16          |
| (1,1510) | 1:66:A:MET:HE3  | 1:42:A:TRP:HE1 | 29       | 0.16          |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1 | 20       | 0.16          |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2 | 20       | 0.16          |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1 | 20       | 0.16          |
| (1,1509) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2 | 20       | 0.16          |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1 | 20       | 0.16          |
| (1,1509) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2 | 20       | 0.16          |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1 | 25       | 0.16          |
| (1,1509) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2 | 25       | 0.16          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 25       | 0.16          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 25       | 0.16          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 25       | 0.16          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 25       | 0.16          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 30       | 0.16          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 30       | 0.16          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 30       | 0.16          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 30       | 0.16          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 30       | 0.16          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 30       | 0.16          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 36       | 0.16          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 36       | 0.16          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 36       | 0.16          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 36       | 0.16          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 36       | 0.16          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 36       | 0.16          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 37       | 0.16          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 37       | 0.16          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 37       | 0.16          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 37       | 0.16          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 37       | 0.16          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 37       | 0.16          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 38       | 0.16          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 38       | 0.16          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 38       | 0.16          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 38       | 0.16          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 38       | 0.16          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 38       | 0.16          |
| (1,1508) | 1:66:A:MET:HE1 | 1:42:A:TRP:HZ3 | 9        | 0.16          |
| (1,1508) | 1:66:A:MET:HE2 | 1:42:A:TRP:HZ3 | 9        | 0.16          |
| (1,1508) | 1:66:A:MET:HE3 | 1:42:A:TRP:HZ3 | 9        | 0.16          |
| (1,1508) | 1:66:A:MET:HE1 | 1:42:A:TRP:HZ3 | 22       | 0.16          |
| (1,1508) | 1:66:A:MET:HE2 | 1:42:A:TRP:HZ3 | 22       | 0.16          |
| (1,1508) | 1:66:A:MET:HE3 | 1:42:A:TRP:HZ3 | 22       | 0.16          |
| (1,1508) | 1:66:A:MET:HE1 | 1:42:A:TRP:HZ3 | 36       | 0.16          |
| (1,1508) | 1:66:A:MET:HE2 | 1:42:A:TRP:HZ3 | 36       | 0.16          |
| (1,1508) | 1:66:A:MET:HE3 | 1:42:A:TRP:HZ3 | 36       | 0.16          |
| (1,1500) | 1:66:A:MET:HE1 | 1:66:A:MET:HB2 | 12       | 0.16          |
| (1,1500) | 1:66:A:MET:HE2 | 1:66:A:MET:HB2 | 12       | 0.16          |
| (1,1500) | 1:66:A:MET:HE3 | 1:66:A:MET:HB2 | 12       | 0.16          |
| (1,1500) | 1:66:A:MET:HE1 | 1:66:A:MET:HB2 | 24       | 0.16          |
| (1,1500) | 1:66:A:MET:HE2 | 1:66:A:MET:HB2 | 24       | 0.16          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1500) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2 | 24       | 0.16          |
| (1,1500) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2 | 33       | 0.16          |
| (1,1500) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2 | 33       | 0.16          |
| (1,1500) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2 | 33       | 0.16          |
| (1,1500) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2 | 40       | 0.16          |
| (1,1500) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2 | 40       | 0.16          |
| (1,1500) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2 | 40       | 0.16          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 9        | 0.16          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 9        | 0.16          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 9        | 0.16          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 10       | 0.16          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 10       | 0.16          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 10       | 0.16          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 20       | 0.16          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 20       | 0.16          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 20       | 0.16          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 23       | 0.16          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 23       | 0.16          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 23       | 0.16          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 32       | 0.16          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 32       | 0.16          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 32       | 0.16          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 40       | 0.16          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 40       | 0.16          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 40       | 0.16          |
| (1,1470) | 1:78:A:VAL:HG21 | 1:79:A:TYR:H   | 29       | 0.16          |
| (1,1470) | 1:78:A:VAL:HG22 | 1:79:A:TYR:H   | 29       | 0.16          |
| (1,1470) | 1:78:A:VAL:HG23 | 1:79:A:TYR:H   | 29       | 0.16          |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 38       | 0.16          |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 38       | 0.16          |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 38       | 0.16          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 10       | 0.16          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 10       | 0.16          |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 10       | 0.16          |
| (1,1462) | 1:71:A:VAL:HG21 | 1:70:A:ASN:H   | 4        | 0.16          |
| (1,1462) | 1:71:A:VAL:HG22 | 1:70:A:ASN:H   | 4        | 0.16          |
| (1,1462) | 1:71:A:VAL:HG23 | 1:70:A:ASN:H   | 4        | 0.16          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H   | 3        | 0.16          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H   | 3        | 0.16          |
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H   | 3        | 0.16          |
| (1,1410) | 1:20:A:VAL:HG11 | 1:20:A:VAL:H   | 12       | 0.16          |
| (1,1410) | 1:20:A:VAL:HG12 | 1:20:A:VAL:H   | 12       | 0.16          |

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| Key      | Atom-1          | Atom-2       | Model ID | Violation (Å) |
|----------|-----------------|--------------|----------|---------------|
| (1,1410) | 1:20:A:VAL:HG13 | 1:20:A:VAL:H | 12       | 0.16          |
| (1,1403) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H | 2        | 0.16          |
| (1,1403) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H | 2        | 0.16          |
| (1,1403) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H | 2        | 0.16          |
| (1,1403) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H | 3        | 0.16          |
| (1,1403) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H | 3        | 0.16          |
| (1,1403) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H | 3        | 0.16          |
| (1,1403) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H | 5        | 0.16          |
| (1,1403) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H | 5        | 0.16          |
| (1,1403) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H | 5        | 0.16          |
| (1,1403) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H | 12       | 0.16          |
| (1,1403) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H | 12       | 0.16          |
| (1,1403) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H | 12       | 0.16          |
| (1,1403) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H | 14       | 0.16          |
| (1,1403) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H | 14       | 0.16          |
| (1,1403) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H | 14       | 0.16          |
| (1,1403) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H | 24       | 0.16          |
| (1,1403) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H | 24       | 0.16          |
| (1,1403) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H | 24       | 0.16          |
| (1,1403) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H | 25       | 0.16          |
| (1,1403) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H | 25       | 0.16          |
| (1,1403) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H | 25       | 0.16          |
| (1,1403) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H | 30       | 0.16          |
| (1,1403) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H | 30       | 0.16          |
| (1,1403) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H | 30       | 0.16          |
| (1,1403) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H | 32       | 0.16          |
| (1,1403) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H | 32       | 0.16          |
| (1,1403) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H | 32       | 0.16          |
| (1,1401) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H | 5        | 0.16          |
| (1,1401) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H | 5        | 0.16          |
| (1,1401) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H | 5        | 0.16          |
| (1,1401) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H | 7        | 0.16          |
| (1,1401) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H | 7        | 0.16          |
| (1,1401) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H | 7        | 0.16          |
| (1,1401) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H | 11       | 0.16          |
| (1,1401) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H | 11       | 0.16          |
| (1,1401) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H | 11       | 0.16          |
| (1,1401) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H | 15       | 0.16          |
| (1,1401) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H | 15       | 0.16          |
| (1,1401) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H | 15       | 0.16          |
| (1,1401) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H | 21       | 0.16          |
| (1,1401) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H | 21       | 0.16          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1401) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 21       | 0.16          |
| (1,1401) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H    | 31       | 0.16          |
| (1,1401) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H    | 31       | 0.16          |
| (1,1401) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 31       | 0.16          |
| (1,1401) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H    | 33       | 0.16          |
| (1,1401) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H    | 33       | 0.16          |
| (1,1401) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 33       | 0.16          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 8        | 0.16          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 8        | 0.16          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 8        | 0.16          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 18       | 0.16          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 18       | 0.16          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 18       | 0.16          |
| (1,1387) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ   | 17       | 0.16          |
| (1,1387) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ   | 17       | 0.16          |
| (1,1387) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ   | 17       | 0.16          |
| (1,1387) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ   | 32       | 0.16          |
| (1,1387) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ   | 32       | 0.16          |
| (1,1387) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ   | 32       | 0.16          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1  | 30       | 0.16          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2  | 30       | 0.16          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3  | 30       | 0.16          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1  | 30       | 0.16          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2  | 30       | 0.16          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3  | 30       | 0.16          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1  | 30       | 0.16          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2  | 30       | 0.16          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3  | 30       | 0.16          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1  | 36       | 0.16          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2  | 36       | 0.16          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3  | 36       | 0.16          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1  | 36       | 0.16          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2  | 36       | 0.16          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3  | 36       | 0.16          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1  | 36       | 0.16          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2  | 36       | 0.16          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3  | 36       | 0.16          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1  | 30       | 0.16          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2  | 30       | 0.16          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3  | 30       | 0.16          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1  | 30       | 0.16          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2  | 30       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1379) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB3  | 30       | 0.16          |
| (1,1379) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB1  | 30       | 0.16          |
| (1,1379) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB2  | 30       | 0.16          |
| (1,1379) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB3  | 30       | 0.16          |
| (1,1379) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB1  | 36       | 0.16          |
| (1,1379) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB2  | 36       | 0.16          |
| (1,1379) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB3  | 36       | 0.16          |
| (1,1379) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB1  | 36       | 0.16          |
| (1,1379) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB2  | 36       | 0.16          |
| (1,1379) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB3  | 36       | 0.16          |
| (1,1379) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB1  | 36       | 0.16          |
| (1,1379) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB2  | 36       | 0.16          |
| (1,1379) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB3  | 36       | 0.16          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 1        | 0.16          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 2        | 0.16          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 4        | 0.16          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 5        | 0.16          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 10       | 0.16          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 17       | 0.16          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 20       | 0.16          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 30       | 0.16          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 35       | 0.16          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 40       | 0.16          |
| (1,1360) | 1:16:A:ILE:HG21 | 1:29:A:PHE:HB2  | 16       | 0.16          |
| (1,1360) | 1:16:A:ILE:HG22 | 1:29:A:PHE:HB2  | 16       | 0.16          |
| (1,1360) | 1:16:A:ILE:HG23 | 1:29:A:PHE:HB2  | 16       | 0.16          |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 5        | 0.16          |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 11       | 0.16          |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 18       | 0.16          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 9        | 0.16          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 9        | 0.16          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 9        | 0.16          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 17       | 0.16          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 17       | 0.16          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 17       | 0.16          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 25       | 0.16          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 25       | 0.16          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 25       | 0.16          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 35       | 0.16          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 35       | 0.16          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 35       | 0.16          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 38       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 38       | 0.16          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 38       | 0.16          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 9        | 0.16          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 9        | 0.16          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 9        | 0.16          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 17       | 0.16          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 17       | 0.16          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 17       | 0.16          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 25       | 0.16          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 25       | 0.16          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 25       | 0.16          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 35       | 0.16          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 35       | 0.16          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 35       | 0.16          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 38       | 0.16          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 38       | 0.16          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 38       | 0.16          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 2        | 0.16          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 2        | 0.16          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 2        | 0.16          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 2        | 0.16          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 2        | 0.16          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 2        | 0.16          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 2        | 0.16          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 2        | 0.16          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 2        | 0.16          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 3        | 0.16          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 3        | 0.16          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 3        | 0.16          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 3        | 0.16          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 3        | 0.16          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 3        | 0.16          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 3        | 0.16          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 3        | 0.16          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 3        | 0.16          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 8        | 0.16          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 8        | 0.16          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 8        | 0.16          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 8        | 0.16          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 8        | 0.16          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 8        | 0.16          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 8        | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 8        | 0.16          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 8        | 0.16          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 10       | 0.16          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 10       | 0.16          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 10       | 0.16          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 10       | 0.16          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 10       | 0.16          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 10       | 0.16          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 10       | 0.16          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 10       | 0.16          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 10       | 0.16          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 15       | 0.16          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 15       | 0.16          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 15       | 0.16          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 15       | 0.16          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 15       | 0.16          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 15       | 0.16          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 15       | 0.16          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 15       | 0.16          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 15       | 0.16          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 19       | 0.16          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 19       | 0.16          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 19       | 0.16          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 19       | 0.16          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 19       | 0.16          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 19       | 0.16          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 19       | 0.16          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 19       | 0.16          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 19       | 0.16          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 26       | 0.16          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 26       | 0.16          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 26       | 0.16          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 26       | 0.16          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 26       | 0.16          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 26       | 0.16          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 26       | 0.16          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 26       | 0.16          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 26       | 0.16          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 27       | 0.16          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 27       | 0.16          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 27       | 0.16          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 27       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 27       | 0.16          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 27       | 0.16          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 27       | 0.16          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 27       | 0.16          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 27       | 0.16          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 6        | 0.16          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 6        | 0.16          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 6        | 0.16          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 28       | 0.16          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 28       | 0.16          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 28       | 0.16          |
| (1,1257) | 1:67:A:THR:HG21 | 1:26:A:SER:HB2  | 7        | 0.16          |
| (1,1257) | 1:67:A:THR:HG22 | 1:26:A:SER:HB2  | 7        | 0.16          |
| (1,1257) | 1:67:A:THR:HG23 | 1:26:A:SER:HB2  | 7        | 0.16          |
| (1,1257) | 1:67:A:THR:HG21 | 1:26:A:SER:HB2  | 31       | 0.16          |
| (1,1257) | 1:67:A:THR:HG22 | 1:26:A:SER:HB2  | 31       | 0.16          |
| (1,1257) | 1:67:A:THR:HG23 | 1:26:A:SER:HB2  | 31       | 0.16          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 1        | 0.16          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 1        | 0.16          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 1        | 0.16          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 8        | 0.16          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 8        | 0.16          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 8        | 0.16          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 17       | 0.16          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 17       | 0.16          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 17       | 0.16          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 25       | 0.16          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 25       | 0.16          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 25       | 0.16          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 38       | 0.16          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 38       | 0.16          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 38       | 0.16          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 10       | 0.16          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 10       | 0.16          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 10       | 0.16          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 14       | 0.16          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 14       | 0.16          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 14       | 0.16          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 26       | 0.16          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 26       | 0.16          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 26       | 0.16          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 36       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 36       | 0.16          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 36       | 0.16          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 37       | 0.16          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 37       | 0.16          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 37       | 0.16          |
| (1,1239) | 1:13:A:THR:HG21 | 1:34:A:SER:H    | 34       | 0.16          |
| (1,1239) | 1:13:A:THR:HG22 | 1:34:A:SER:H    | 34       | 0.16          |
| (1,1239) | 1:13:A:THR:HG23 | 1:34:A:SER:H    | 34       | 0.16          |
| (1,1236) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3  | 17       | 0.16          |
| (1,1236) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3  | 17       | 0.16          |
| (1,1236) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3  | 17       | 0.16          |
| (1,1217) | 1:69:A:HIS:H    | 1:56:A:ASN:H    | 19       | 0.16          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 2        | 0.16          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 2        | 0.16          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 2        | 0.16          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 11       | 0.16          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 11       | 0.16          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 11       | 0.16          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 36       | 0.16          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 36       | 0.16          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 36       | 0.16          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 3        | 0.16          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 3        | 0.16          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 3        | 0.16          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 21       | 0.16          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 21       | 0.16          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 21       | 0.16          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 29       | 0.16          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 29       | 0.16          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 29       | 0.16          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 31       | 0.16          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 31       | 0.16          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 31       | 0.16          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 32       | 0.16          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 32       | 0.16          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 32       | 0.16          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 38       | 0.16          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 38       | 0.16          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 38       | 0.16          |
| (1,1185) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 4        | 0.16          |
| (1,1177) | 1:100:A:GLU:H   | 1:21:A:VAL:HG11 | 9        | 0.16          |
| (1,1177) | 1:100:A:GLU:H   | 1:21:A:VAL:HG12 | 9        | 0.16          |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1177) | 1:100:A:GLU:H | 1:21:A:VAL:HG13 | 9        | 0.16          |
| (1,1176) | 1:47:A:THR:H  | 1:44:A:LYS:HB3  | 19       | 0.16          |
| (1,1174) | 1:91:A:ALA:H  | 1:84:A:ARG:HA   | 1        | 0.16          |
| (1,1174) | 1:91:A:ALA:H  | 1:84:A:ARG:HA   | 17       | 0.16          |
| (1,1174) | 1:91:A:ALA:H  | 1:84:A:ARG:HA   | 18       | 0.16          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 1        | 0.16          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 1        | 0.16          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 2        | 0.16          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 2        | 0.16          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 20       | 0.16          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 20       | 0.16          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 27       | 0.16          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 27       | 0.16          |
| (1,1149) | 1:54:A:LYS:H  | 1:53:A:GLN:HG3  | 22       | 0.16          |
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 4        | 0.16          |
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 40       | 0.16          |
| (1,1125) | 1:78:A:VAL:H  | 1:44:A:LYS:HE2  | 20       | 0.16          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 5        | 0.16          |
| (1,1020) | 1:48:A:GLU:H  | 1:48:A:GLU:HG3  | 12       | 0.16          |
| (1,1020) | 1:48:A:GLU:H  | 1:48:A:GLU:HG3  | 15       | 0.16          |
| (1,1020) | 1:48:A:GLU:H  | 1:48:A:GLU:HG3  | 39       | 0.16          |
| (1,987)  | 1:12:A:PHE:H  | 1:11:A:GLN:HB2  | 1        | 0.16          |
| (1,967)  | 1:21:A:VAL:H  | 1:99:A:GLY:HA3  | 6        | 0.16          |
| (1,967)  | 1:21:A:VAL:H  | 1:99:A:GLY:HA3  | 9        | 0.16          |
| (1,967)  | 1:21:A:VAL:H  | 1:99:A:GLY:HA3  | 11       | 0.16          |
| (1,941)  | 1:34:A:SER:H  | 1:12:A:PHE:HA   | 34       | 0.16          |
| (1,933)  | 1:98:A:LYS:H  | 1:20:A:VAL:HG11 | 19       | 0.16          |
| (1,933)  | 1:98:A:LYS:H  | 1:20:A:VAL:HG12 | 19       | 0.16          |
| (1,933)  | 1:98:A:LYS:H  | 1:20:A:VAL:HG13 | 19       | 0.16          |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 2        | 0.16          |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 11       | 0.16          |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 20       | 0.16          |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 25       | 0.16          |
| (1,932)  | 1:98:A:LYS:H  | 1:19:A:ILE:HB   | 27       | 0.16          |
| (1,919)  | 1:37:A:ASP:H  | 1:36:A:ASP:HB2  | 31       | 0.16          |
| (1,888)  | 1:80:A:SER:H  | 1:43:A:TYR:HB3  | 2        | 0.16          |
| (1,888)  | 1:80:A:SER:H  | 1:43:A:TYR:HB3  | 17       | 0.16          |
| (1,888)  | 1:80:A:SER:H  | 1:43:A:TYR:HB3  | 22       | 0.16          |
| (1,888)  | 1:80:A:SER:H  | 1:43:A:TYR:HB3  | 25       | 0.16          |
| (1,888)  | 1:80:A:SER:H  | 1:43:A:TYR:HB3  | 29       | 0.16          |
| (1,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3   | 7        | 0.16          |
| (1,871)  | 1:8:A:GLU:H   | 1:9:A:PRO:HD3   | 10       | 0.16          |

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| Key     | Atom-1       | Atom-2         | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (1,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3  | 11       | 0.16          |
| (1,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3  | 15       | 0.16          |
| (1,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3  | 20       | 0.16          |
| (1,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3  | 21       | 0.16          |
| (1,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2  | 32       | 0.16          |
| (1,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2  | 33       | 0.16          |
| (1,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2  | 36       | 0.16          |
| (1,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA   | 11       | 0.16          |
| (1,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA   | 12       | 0.16          |
| (1,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA   | 14       | 0.16          |
| (1,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA   | 17       | 0.16          |
| (1,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA   | 23       | 0.16          |
| (1,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA   | 25       | 0.16          |
| (1,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA   | 28       | 0.16          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1 | 5        | 0.16          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2 | 5        | 0.16          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3 | 5        | 0.16          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 1        | 0.16          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 2        | 0.16          |
| (1,847) | 1:83:A:ALA:H | 1:83:A:ALA:HA  | 15       | 0.16          |
| (1,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB  | 10       | 0.16          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2 | 3        | 0.16          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2 | 10       | 0.16          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2 | 24       | 0.16          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2 | 27       | 0.16          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2 | 29       | 0.16          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2 | 33       | 0.16          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2 | 38       | 0.16          |
| (1,801) | 1:54:A:LYS:H | 1:54:A:LYS:HD2 | 40       | 0.16          |
| (1,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 1        | 0.16          |
| (1,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 4        | 0.16          |
| (1,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 6        | 0.16          |
| (1,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 10       | 0.16          |
| (1,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 13       | 0.16          |
| (1,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 15       | 0.16          |
| (1,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 17       | 0.16          |
| (1,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 18       | 0.16          |
| (1,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 23       | 0.16          |
| (1,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 24       | 0.16          |
| (1,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 29       | 0.16          |
| (1,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 31       | 0.16          |
| (1,717) | 1:16:A:ILE:H | 1:15:A:ARG:HB2 | 39       | 0.16          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 4        | 0.16          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 6        | 0.16          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 15       | 0.16          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 29       | 0.16          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 33       | 0.16          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 29       | 0.16          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 34       | 0.16          |
| (1,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 1        | 0.16          |
| (1,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 2        | 0.16          |
| (1,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 5        | 0.16          |
| (1,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 8        | 0.16          |
| (1,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 10       | 0.16          |
| (1,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 12       | 0.16          |
| (1,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 14       | 0.16          |
| (1,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 16       | 0.16          |
| (1,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 29       | 0.16          |
| (1,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 39       | 0.16          |
| (1,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 40       | 0.16          |
| (1,591) | 1:3:A:ASP:H   | 1:3:A:ASP:HA    | 13       | 0.16          |
| (1,591) | 1:3:A:ASP:H   | 1:3:A:ASP:HA    | 34       | 0.16          |
| (1,560) | 1:47:A:THR:H  | 1:47:A:THR:HA   | 4        | 0.16          |
| (1,560) | 1:47:A:THR:H  | 1:47:A:THR:HA   | 8        | 0.16          |
| (1,560) | 1:47:A:THR:H  | 1:47:A:THR:HA   | 14       | 0.16          |
| (1,560) | 1:47:A:THR:H  | 1:47:A:THR:HA   | 15       | 0.16          |
| (1,560) | 1:47:A:THR:H  | 1:47:A:THR:HA   | 16       | 0.16          |
| (1,560) | 1:47:A:THR:H  | 1:47:A:THR:HA   | 27       | 0.16          |
| (1,560) | 1:47:A:THR:H  | 1:47:A:THR:HA   | 28       | 0.16          |
| (1,560) | 1:47:A:THR:H  | 1:47:A:THR:HA   | 38       | 0.16          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 2        | 0.16          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2  | 2        | 0.16          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 8        | 0.16          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2  | 8        | 0.16          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 21       | 0.16          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2  | 21       | 0.16          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 22       | 0.16          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2  | 22       | 0.16          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 33       | 0.16          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2  | 33       | 0.16          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 34       | 0.16          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2  | 34       | 0.16          |
| (1,546) | 1:71:A:VAL:H  | 1:24:A:HIS:HA   | 15       | 0.16          |
| (1,531) | 1:99:A:GLY:H  | 1:98:A:LYS:HG2  | 4        | 0.16          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 15       | 0.16          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 16       | 0.16          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 38       | 0.16          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 39       | 0.16          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 40       | 0.16          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 4        | 0.16          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 33       | 0.16          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 35       | 0.16          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 38       | 0.16          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 39       | 0.16          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 1        | 0.16          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 12       | 0.16          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 17       | 0.16          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 28       | 0.16          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 29       | 0.16          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 30       | 0.16          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 18       | 0.16          |
| (1,525) | 1:99:A:GLY:H | 1:100:A:GLU:H   | 31       | 0.16          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 22       | 0.16          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 31       | 0.16          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 34       | 0.16          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 36       | 0.16          |
| (1,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 9        | 0.16          |
| (1,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 19       | 0.16          |
| (1,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 28       | 0.16          |
| (1,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 31       | 0.16          |
| (1,410) | 1:96:A:GLU:H | 1:18:A:ASN:HD21 | 17       | 0.16          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 8        | 0.16          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 13       | 0.16          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 15       | 0.16          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 22       | 0.16          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 23       | 0.16          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 25       | 0.16          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 26       | 0.16          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 29       | 0.16          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 30       | 0.16          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 35       | 0.16          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 38       | 0.16          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 39       | 0.16          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 22       | 0.16          |
| (1,393) | 1:77:A:GLY:H | 1:96:A:GLU:HA   | 20       | 0.16          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 5        | 0.16          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 5        | 0.16          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 5        | 0.16          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 8        | 0.16          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 8        | 0.16          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 8        | 0.16          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 10       | 0.16          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 10       | 0.16          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 10       | 0.16          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 14       | 0.16          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 14       | 0.16          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 14       | 0.16          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 30       | 0.16          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 30       | 0.16          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 30       | 0.16          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 31       | 0.16          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 31       | 0.16          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 31       | 0.16          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 2        | 0.16          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 2        | 0.16          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 2        | 0.16          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 3        | 0.16          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 3        | 0.16          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 3        | 0.16          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 5        | 0.16          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 5        | 0.16          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 5        | 0.16          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 12       | 0.16          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 12       | 0.16          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 12       | 0.16          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 14       | 0.16          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 14       | 0.16          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 14       | 0.16          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 24       | 0.16          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 24       | 0.16          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 24       | 0.16          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 25       | 0.16          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 25       | 0.16          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 25       | 0.16          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 30       | 0.16          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 30       | 0.16          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 30       | 0.16          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 32       | 0.16          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,370) | 1:18:A:ASN:H  | 1:95:A:ALA:HB2  | 32       | 0.16          |
| (1,370) | 1:18:A:ASN:H  | 1:95:A:ALA:HB3  | 32       | 0.16          |
| (1,368) | 1:18:A:ASN:H  | 1:17:A:GLN:HB3  | 29       | 0.16          |
| (1,343) | 1:14:A:LYS:H  | 1:33:A:VAL:HA   | 9        | 0.16          |
| (1,343) | 1:14:A:LYS:H  | 1:33:A:VAL:HA   | 13       | 0.16          |
| (1,314) | 1:63:A:CYS:H  | 1:64:A:HIS:HD2  | 31       | 0.16          |
| (1,296) | 1:31:A:CYS:H  | 1:30:A:GLU:HB3  | 1        | 0.16          |
| (1,296) | 1:31:A:CYS:H  | 1:30:A:GLU:HB3  | 11       | 0.16          |
| (1,296) | 1:31:A:CYS:H  | 1:30:A:GLU:HB3  | 22       | 0.16          |
| (1,296) | 1:31:A:CYS:H  | 1:30:A:GLU:HB3  | 25       | 0.16          |
| (1,296) | 1:31:A:CYS:H  | 1:30:A:GLU:HB3  | 30       | 0.16          |
| (1,296) | 1:31:A:CYS:H  | 1:30:A:GLU:HB3  | 36       | 0.16          |
| (1,296) | 1:31:A:CYS:H  | 1:30:A:GLU:HB3  | 37       | 0.16          |
| (1,274) | 1:66:A:MET:H  | 1:66:A:MET:HG3  | 10       | 0.16          |
| (1,274) | 1:66:A:MET:H  | 1:66:A:MET:HG3  | 16       | 0.16          |
| (1,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 1        | 0.16          |
| (1,235) | 1:13:A:THR:H  | 1:12:A:PHE:HB2  | 9        | 0.16          |
| (1,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD1  | 12       | 0.16          |
| (1,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD2  | 12       | 0.16          |
| (1,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 4        | 0.16          |
| (1,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 16       | 0.16          |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG21 | 24       | 0.16          |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG22 | 24       | 0.16          |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG23 | 24       | 0.16          |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG21 | 27       | 0.16          |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG22 | 27       | 0.16          |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG23 | 27       | 0.16          |
| (1,198) | 1:90:A:GLU:H  | 1:90:A:GLU:HB2  | 21       | 0.16          |
| (1,198) | 1:90:A:GLU:H  | 1:90:A:GLU:HB2  | 24       | 0.16          |
| (1,198) | 1:90:A:GLU:H  | 1:90:A:GLU:HB2  | 25       | 0.16          |
| (1,198) | 1:90:A:GLU:H  | 1:90:A:GLU:HB2  | 32       | 0.16          |
| (1,198) | 1:90:A:GLU:H  | 1:90:A:GLU:HB2  | 35       | 0.16          |
| (1,198) | 1:90:A:GLU:H  | 1:90:A:GLU:HB2  | 40       | 0.16          |
| (1,148) | 1:45:A:GLY:H  | 1:46:A:PRO:HD2  | 26       | 0.16          |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 4        | 0.16          |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 40       | 0.16          |
| (1,133) | 1:39:A:ILE:H  | 1:39:A:ILE:HG13 | 7        | 0.16          |
| (1,70)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 1        | 0.16          |
| (1,70)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 5        | 0.16          |
| (1,70)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 8        | 0.16          |
| (1,70)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 10       | 0.16          |
| (1,70)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 13       | 0.16          |

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| Key    | Atom-1       | Atom-2         | Model ID | Violation (Å) |
|--------|--------------|----------------|----------|---------------|
| (1,70) | 1:51:A:GLU:H | 1:51:A:GLU:HG2 | 16       | 0.16          |
| (1,70) | 1:51:A:GLU:H | 1:51:A:GLU:HG2 | 20       | 0.16          |
| (1,70) | 1:51:A:GLU:H | 1:51:A:GLU:HG2 | 37       | 0.16          |
| (1,57) | 1:42:A:TRP:H | 1:41:A:THR:HB  | 10       | 0.16          |
| (1,57) | 1:42:A:TRP:H | 1:41:A:THR:HB  | 11       | 0.16          |
| (1,57) | 1:42:A:TRP:H | 1:41:A:THR:HB  | 12       | 0.16          |
| (1,57) | 1:42:A:TRP:H | 1:41:A:THR:HB  | 13       | 0.16          |
| (1,57) | 1:42:A:TRP:H | 1:41:A:THR:HB  | 14       | 0.16          |
| (1,57) | 1:42:A:TRP:H | 1:41:A:THR:HB  | 20       | 0.16          |
| (1,57) | 1:42:A:TRP:H | 1:41:A:THR:HB  | 21       | 0.16          |
| (1,57) | 1:42:A:TRP:H | 1:41:A:THR:HB  | 23       | 0.16          |
| (1,57) | 1:42:A:TRP:H | 1:41:A:THR:HB  | 24       | 0.16          |
| (1,57) | 1:42:A:TRP:H | 1:41:A:THR:HB  | 35       | 0.16          |
| (1,57) | 1:42:A:TRP:H | 1:41:A:THR:HB  | 36       | 0.16          |
| (1,49) | 1:57:A:PHE:H | 1:56:A:ASN:HB2 | 7        | 0.16          |
| (1,49) | 1:57:A:PHE:H | 1:56:A:ASN:HB2 | 14       | 0.16          |
| (1,49) | 1:57:A:PHE:H | 1:56:A:ASN:HB2 | 17       | 0.16          |
| (1,49) | 1:57:A:PHE:H | 1:56:A:ASN:HB2 | 25       | 0.16          |
| (1,35) | 1:88:A:ARG:H | 1:88:A:ARG:HG2 | 9        | 0.16          |
| (1,25) | 1:89:A:GLY:H | 1:88:A:ARG:HB3 | 4        | 0.16          |
| (1,25) | 1:89:A:GLY:H | 1:88:A:ARG:HB3 | 5        | 0.16          |
| (1,22) | 1:89:A:GLY:H | 1:85:A:LEU:H   | 1        | 0.16          |
| (1,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 1        | 0.16          |
| (1,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 2        | 0.16          |
| (1,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 3        | 0.16          |
| (1,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 4        | 0.16          |
| (1,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 5        | 0.16          |
| (1,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 7        | 0.16          |
| (1,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 8        | 0.16          |
| (1,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 9        | 0.16          |
| (1,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 10       | 0.16          |
| (1,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 12       | 0.16          |
| (1,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 13       | 0.16          |
| (1,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 14       | 0.16          |
| (1,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 16       | 0.16          |
| (1,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 17       | 0.16          |
| (1,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 20       | 0.16          |
| (1,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 21       | 0.16          |
| (1,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 22       | 0.16          |
| (1,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 23       | 0.16          |
| (1,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 24       | 0.16          |
| (1,18) | 1:89:A:GLY:H | 1:89:A:GLY:HA3 | 25       | 0.16          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 26       | 0.16          |
| (1,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 27       | 0.16          |
| (1,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 28       | 0.16          |
| (1,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 30       | 0.16          |
| (1,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 32       | 0.16          |
| (1,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 34       | 0.16          |
| (1,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 35       | 0.16          |
| (1,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 37       | 0.16          |
| (1,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 38       | 0.16          |
| (1,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 39       | 0.16          |
| (1,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 40       | 0.16          |
| (3,3217) | 1:69:A:HIS:HE1 | 1:67:A:THR:HB   | 15       | 0.15          |
| (3,3217) | 1:69:A:HIS:HE1 | 1:67:A:THR:HB   | 22       | 0.15          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 17       | 0.15          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 17       | 0.15          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 18       | 0.15          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 18       | 0.15          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 5        | 0.15          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 5        | 0.15          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 5        | 0.15          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 5        | 0.15          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 5        | 0.15          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 5        | 0.15          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 7        | 0.15          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 7        | 0.15          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 7        | 0.15          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 7        | 0.15          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 7        | 0.15          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 7        | 0.15          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 11       | 0.15          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 11       | 0.15          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 11       | 0.15          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 11       | 0.15          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 11       | 0.15          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 11       | 0.15          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 14       | 0.15          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 14       | 0.15          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 14       | 0.15          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 14       | 0.15          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 14       | 0.15          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 14       | 0.15          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 15       | 0.15          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 15       | 0.15          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 15       | 0.15          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 15       | 0.15          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 15       | 0.15          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 15       | 0.15          |
| (3,3205) | 1:43:A:TYR:HD1 | 1:80:A:SER:HB2  | 29       | 0.15          |
| (3,3205) | 1:43:A:TYR:HD2 | 1:80:A:SER:HB2  | 29       | 0.15          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 16       | 0.15          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 16       | 0.15          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 16       | 0.15          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 16       | 0.15          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 21       | 0.15          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 21       | 0.15          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 21       | 0.15          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 21       | 0.15          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 28       | 0.15          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 28       | 0.15          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 28       | 0.15          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 28       | 0.15          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 39       | 0.15          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 39       | 0.15          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 39       | 0.15          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 39       | 0.15          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 40       | 0.15          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 40       | 0.15          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 40       | 0.15          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 40       | 0.15          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 37       | 0.15          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 40       | 0.15          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 15       | 0.15          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 15       | 0.15          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 15       | 0.15          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 19       | 0.15          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 19       | 0.15          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 19       | 0.15          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 21       | 0.15          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 21       | 0.15          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 21       | 0.15          |
| (3,3143) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3  | 1        | 0.15          |
| (3,3143) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 1        | 0.15          |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2  | 11       | 0.15          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2  | 11       | 0.15          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 16       | 0.15          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 16       | 0.15          |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 26       | 0.15          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 26       | 0.15          |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 27       | 0.15          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 27       | 0.15          |
| (3,3138) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB2 | 10       | 0.15          |
| (3,3138) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB2 | 10       | 0.15          |
| (3,3137) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3 | 1        | 0.15          |
| (3,3137) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3 | 1        | 0.15          |
| (3,3137) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3 | 7        | 0.15          |
| (3,3137) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3 | 7        | 0.15          |
| (3,3137) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3 | 36       | 0.15          |
| (3,3137) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3 | 36       | 0.15          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 4        | 0.15          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 4        | 0.15          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 12       | 0.15          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 12       | 0.15          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 13       | 0.15          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 13       | 0.15          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 14       | 0.15          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 14       | 0.15          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 15       | 0.15          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 15       | 0.15          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 17       | 0.15          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 17       | 0.15          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 19       | 0.15          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 19       | 0.15          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 25       | 0.15          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 25       | 0.15          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 30       | 0.15          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 30       | 0.15          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 36       | 0.15          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 36       | 0.15          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 37       | 0.15          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 37       | 0.15          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 4        | 0.15          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 4        | 0.15          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 12       | 0.15          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 12       | 0.15          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 13       | 0.15          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 13       | 0.15          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 14       | 0.15          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 14       | 0.15          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 15       | 0.15          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 15       | 0.15          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 17       | 0.15          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 17       | 0.15          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 19       | 0.15          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 19       | 0.15          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 25       | 0.15          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 25       | 0.15          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 30       | 0.15          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 30       | 0.15          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 36       | 0.15          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 36       | 0.15          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 37       | 0.15          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 37       | 0.15          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 2        | 0.15          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 2        | 0.15          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 2        | 0.15          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 2        | 0.15          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 2        | 0.15          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 2        | 0.15          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 4        | 0.15          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 4        | 0.15          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 4        | 0.15          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 4        | 0.15          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 4        | 0.15          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 4        | 0.15          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 31       | 0.15          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 31       | 0.15          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 31       | 0.15          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 31       | 0.15          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 31       | 0.15          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 31       | 0.15          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 32       | 0.15          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 32       | 0.15          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 32       | 0.15          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 32       | 0.15          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 32       | 0.15          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 32       | 0.15          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 34       | 0.15          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 34       | 0.15          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 34       | 0.15          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 34       | 0.15          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 34       | 0.15          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 34       | 0.15          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 36       | 0.15          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 36       | 0.15          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 36       | 0.15          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 36       | 0.15          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 36       | 0.15          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 36       | 0.15          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 37       | 0.15          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 37       | 0.15          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 37       | 0.15          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 37       | 0.15          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 37       | 0.15          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 37       | 0.15          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 11       | 0.15          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 11       | 0.15          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 11       | 0.15          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 11       | 0.15          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 11       | 0.15          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 11       | 0.15          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 17       | 0.15          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 17       | 0.15          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 17       | 0.15          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 17       | 0.15          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 17       | 0.15          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 17       | 0.15          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 25       | 0.15          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 25       | 0.15          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 25       | 0.15          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 25       | 0.15          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 25       | 0.15          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 25       | 0.15          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 27       | 0.15          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 27       | 0.15          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 27       | 0.15          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 27       | 0.15          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 27       | 0.15          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 27       | 0.15          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 30       | 0.15          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 30       | 0.15          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 30       | 0.15          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 30       | 0.15          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 30       | 0.15          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 30       | 0.15          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 8        | 0.15          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 8        | 0.15          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 8        | 0.15          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 8        | 0.15          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 22       | 0.15          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 22       | 0.15          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 22       | 0.15          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 22       | 0.15          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 37       | 0.15          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 37       | 0.15          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 37       | 0.15          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 37       | 0.15          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 7        | 0.15          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 7        | 0.15          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 7        | 0.15          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 7        | 0.15          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 7        | 0.15          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 7        | 0.15          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 9        | 0.15          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 9        | 0.15          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 9        | 0.15          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 9        | 0.15          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 9        | 0.15          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 9        | 0.15          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 10       | 0.15          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 10       | 0.15          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 10       | 0.15          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 10       | 0.15          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 10       | 0.15          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 10       | 0.15          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 16       | 0.15          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 16       | 0.15          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 16       | 0.15          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 16       | 0.15          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 16       | 0.15          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 16       | 0.15          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 24       | 0.15          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 24       | 0.15          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 24       | 0.15          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 24       | 0.15          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 24       | 0.15          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 24       | 0.15          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 39       | 0.15          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 39       | 0.15          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 39       | 0.15          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 39       | 0.15          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 39       | 0.15          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 39       | 0.15          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 10       | 0.15          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 10       | 0.15          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 10       | 0.15          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 24       | 0.15          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 24       | 0.15          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 24       | 0.15          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 31       | 0.15          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 31       | 0.15          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 31       | 0.15          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 1        | 0.15          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 1        | 0.15          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 3        | 0.15          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 3        | 0.15          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 17       | 0.15          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 17       | 0.15          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 22       | 0.15          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 22       | 0.15          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 26       | 0.15          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 26       | 0.15          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 31       | 0.15          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 31       | 0.15          |
| (3,3048) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG21 | 10       | 0.15          |
| (3,3048) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG22 | 10       | 0.15          |
| (3,3048) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG23 | 10       | 0.15          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 22       | 0.15          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 22       | 0.15          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 22       | 0.15          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 23       | 0.15          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 23       | 0.15          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 23       | 0.15          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 31       | 0.15          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 31       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,3020) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG23 | 31       | 0.15          |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG21 | 19       | 0.15          |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG22 | 19       | 0.15          |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG23 | 19       | 0.15          |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG21 | 26       | 0.15          |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG22 | 26       | 0.15          |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG23 | 26       | 0.15          |
| (3,3004) | 1:15:A:ARG:HG2  | 1:93:A:SER:HB3  | 10       | 0.15          |
| (3,3004) | 1:15:A:ARG:HG2  | 1:93:A:SER:HB3  | 15       | 0.15          |
| (3,3004) | 1:15:A:ARG:HG2  | 1:93:A:SER:HB3  | 27       | 0.15          |
| (3,2982) | 1:65:A:TYR:HA   | 1:42:A:TRP:HZ2  | 15       | 0.15          |
| (3,2982) | 1:65:A:TYR:HA   | 1:42:A:TRP:HZ2  | 16       | 0.15          |
| (3,2970) | 1:44:A:LYS:HE2  | 1:44:A:LYS:HG3  | 35       | 0.15          |
| (3,2957) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 3        | 0.15          |
| (3,2957) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 25       | 0.15          |
| (3,2944) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD1  | 1        | 0.15          |
| (3,2944) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD2  | 1        | 0.15          |
| (3,2938) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 3        | 0.15          |
| (3,2938) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 25       | 0.15          |
| (3,2936) | 1:17:A:GLN:HG2  | 1:17:A:GLN:H    | 5        | 0.15          |
| (3,2936) | 1:17:A:GLN:HG2  | 1:17:A:GLN:H    | 26       | 0.15          |
| (3,2925) | 1:22:A:SER:HB2  | 1:25:A:GLN:H    | 34       | 0.15          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 2        | 0.15          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 3        | 0.15          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 5        | 0.15          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 14       | 0.15          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 15       | 0.15          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 22       | 0.15          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 2        | 0.15          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 4        | 0.15          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 6        | 0.15          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 11       | 0.15          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 13       | 0.15          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 19       | 0.15          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 22       | 0.15          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 23       | 0.15          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 31       | 0.15          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 37       | 0.15          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 9        | 0.15          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 16       | 0.15          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 24       | 0.15          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 34       | 0.15          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H | 39       | 0.15          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H | 40       | 0.15          |
| (3,2761) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H  | 3        | 0.15          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 1        | 0.15          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 2        | 0.15          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 10       | 0.15          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 11       | 0.15          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 18       | 0.15          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 21       | 0.15          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 24       | 0.15          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 31       | 0.15          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 32       | 0.15          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 33       | 0.15          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 34       | 0.15          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 40       | 0.15          |
| (3,2690) | 1:8:A:GLU:HB3   | 1:8:A:GLU:HG2 | 1        | 0.15          |
| (3,2690) | 1:8:A:GLU:HB3   | 1:8:A:GLU:HG2 | 11       | 0.15          |
| (3,2690) | 1:8:A:GLU:HB3   | 1:8:A:GLU:HG2 | 23       | 0.15          |
| (3,2690) | 1:8:A:GLU:HB3   | 1:8:A:GLU:HG2 | 32       | 0.15          |
| (3,2679) | 1:25:A:GLN:HG3  | 1:26:A:SER:H  | 3        | 0.15          |
| (3,2679) | 1:25:A:GLN:HG3  | 1:26:A:SER:H  | 16       | 0.15          |
| (3,2679) | 1:25:A:GLN:HG3  | 1:26:A:SER:H  | 21       | 0.15          |
| (3,2679) | 1:25:A:GLN:HG3  | 1:26:A:SER:H  | 25       | 0.15          |
| (3,2679) | 1:25:A:GLN:HG3  | 1:26:A:SER:H  | 29       | 0.15          |
| (3,2679) | 1:25:A:GLN:HG3  | 1:26:A:SER:H  | 33       | 0.15          |
| (3,2679) | 1:25:A:GLN:HG3  | 1:26:A:SER:H  | 34       | 0.15          |
| (3,2679) | 1:25:A:GLN:HG3  | 1:26:A:SER:H  | 35       | 0.15          |
| (3,2679) | 1:25:A:GLN:HG3  | 1:26:A:SER:H  | 36       | 0.15          |
| (3,2679) | 1:25:A:GLN:HG3  | 1:26:A:SER:H  | 38       | 0.15          |
| (3,2657) | 1:17:A:GLN:HG2  | 1:17:A:GLN:HA | 8        | 0.15          |
| (3,2650) | 1:9:A:PRO:HB2   | 1:9:A:PRO:HD3 | 28       | 0.15          |
| (3,2554) | 1:92:A:ARG:HA   | 1:83:A:ALA:H  | 23       | 0.15          |
| (3,2554) | 1:92:A:ARG:HA   | 1:83:A:ALA:H  | 27       | 0.15          |
| (3,2554) | 1:92:A:ARG:HA   | 1:83:A:ALA:H  | 40       | 0.15          |
| (3,2543) | 1:73:A:PRO:HG2  | 1:73:A:PRO:HA | 1        | 0.15          |
| (3,2543) | 1:73:A:PRO:HG2  | 1:73:A:PRO:HA | 3        | 0.15          |
| (3,2543) | 1:73:A:PRO:HG2  | 1:73:A:PRO:HA | 5        | 0.15          |
| (3,2543) | 1:73:A:PRO:HG2  | 1:73:A:PRO:HA | 9        | 0.15          |
| (3,2543) | 1:73:A:PRO:HG2  | 1:73:A:PRO:HA | 10       | 0.15          |
| (3,2543) | 1:73:A:PRO:HG2  | 1:73:A:PRO:HA | 13       | 0.15          |
| (3,2543) | 1:73:A:PRO:HG2  | 1:73:A:PRO:HA | 14       | 0.15          |
| (3,2543) | 1:73:A:PRO:HG2  | 1:73:A:PRO:HA | 19       | 0.15          |

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| Key      | Atom-1         | Atom-2        | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (3,2541) | 1:73:A:PRO:HG3 | 1:73:A:PRO:HA | 23       | 0.15          |
| (3,2541) | 1:73:A:PRO:HG3 | 1:73:A:PRO:HA | 37       | 0.15          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 1        | 0.15          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 2        | 0.15          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 3        | 0.15          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 4        | 0.15          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 5        | 0.15          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 6        | 0.15          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 7        | 0.15          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 9        | 0.15          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 10       | 0.15          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 11       | 0.15          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 12       | 0.15          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 13       | 0.15          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 14       | 0.15          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 15       | 0.15          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 16       | 0.15          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 18       | 0.15          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 19       | 0.15          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 20       | 0.15          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 1        | 0.15          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 2        | 0.15          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 4        | 0.15          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 8        | 0.15          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 9        | 0.15          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 10       | 0.15          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 13       | 0.15          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 15       | 0.15          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 16       | 0.15          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 17       | 0.15          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 18       | 0.15          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 19       | 0.15          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 20       | 0.15          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3 | 2        | 0.15          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3 | 7        | 0.15          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3 | 9        | 0.15          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3 | 10       | 0.15          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3 | 11       | 0.15          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3 | 12       | 0.15          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3 | 13       | 0.15          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3 | 15       | 0.15          |
| (3,2488) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HB3 | 18       | 0.15          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (3,2488) | 1:9:A:PRO:HD2 | 1:9:A:PRO:HB3 | 20       | 0.15          |
| (3,2482) | 1:9:A:PRO:HD2 | 1:8:A:GLU:HA  | 2        | 0.15          |
| (3,2482) | 1:9:A:PRO:HD2 | 1:8:A:GLU:HA  | 10       | 0.15          |
| (3,2482) | 1:9:A:PRO:HD2 | 1:8:A:GLU:HA  | 18       | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 2        | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 3        | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 5        | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 6        | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 7        | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 8        | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 11       | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 13       | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 14       | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 19       | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 20       | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 21       | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 22       | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 23       | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 24       | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 25       | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 26       | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 27       | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 28       | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 29       | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 30       | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 31       | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 32       | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 33       | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 34       | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 36       | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 37       | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 38       | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 39       | 0.15          |
| (3,2478) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 40       | 0.15          |
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 2        | 0.15          |
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 3        | 0.15          |
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 5        | 0.15          |
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 6        | 0.15          |
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 7        | 0.15          |
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 8        | 0.15          |
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 11       | 0.15          |
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 13       | 0.15          |

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| Key      | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|----------|---------------|----------------|----------|---------------|
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3  | 14       | 0.15          |
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3  | 19       | 0.15          |
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3  | 20       | 0.15          |
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3  | 21       | 0.15          |
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3  | 22       | 0.15          |
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3  | 23       | 0.15          |
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3  | 24       | 0.15          |
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3  | 25       | 0.15          |
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3  | 26       | 0.15          |
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3  | 27       | 0.15          |
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3  | 28       | 0.15          |
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3  | 29       | 0.15          |
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3  | 30       | 0.15          |
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3  | 31       | 0.15          |
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3  | 32       | 0.15          |
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3  | 33       | 0.15          |
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3  | 34       | 0.15          |
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3  | 36       | 0.15          |
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3  | 37       | 0.15          |
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3  | 38       | 0.15          |
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3  | 39       | 0.15          |
| (3,2477) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3  | 40       | 0.15          |
| (3,2463) | 1:4:A:PRO:HD3 | 1:3:A:ASP:HA   | 14       | 0.15          |
| (3,2463) | 1:4:A:PRO:HD3 | 1:3:A:ASP:HA   | 23       | 0.15          |
| (3,2434) | 1:82:A:ILE:HB | 1:41:A:THR:H   | 4        | 0.15          |
| (3,2434) | 1:82:A:ILE:HB | 1:41:A:THR:H   | 21       | 0.15          |
| (3,2434) | 1:82:A:ILE:HB | 1:41:A:THR:H   | 22       | 0.15          |
| (3,2434) | 1:82:A:ILE:HB | 1:41:A:THR:H   | 24       | 0.15          |
| (3,2434) | 1:82:A:ILE:HB | 1:41:A:THR:H   | 25       | 0.15          |
| (3,2419) | 1:10:A:ILE:HB | 1:9:A:PRO:HA   | 32       | 0.15          |
| (3,2412) | 1:10:A:ILE:HA | 1:11:A:GLN:HG2 | 4        | 0.15          |
| (3,2412) | 1:10:A:ILE:HA | 1:11:A:GLN:HG2 | 6        | 0.15          |
| (3,2412) | 1:10:A:ILE:HA | 1:11:A:GLN:HG2 | 11       | 0.15          |
| (3,2412) | 1:10:A:ILE:HA | 1:11:A:GLN:HG2 | 12       | 0.15          |
| (3,2412) | 1:10:A:ILE:HA | 1:11:A:GLN:HG2 | 14       | 0.15          |
| (3,2412) | 1:10:A:ILE:HA | 1:11:A:GLN:HG2 | 16       | 0.15          |
| (3,2412) | 1:10:A:ILE:HA | 1:11:A:GLN:HG2 | 20       | 0.15          |
| (3,2412) | 1:10:A:ILE:HA | 1:11:A:GLN:HG2 | 21       | 0.15          |
| (3,2412) | 1:10:A:ILE:HA | 1:11:A:GLN:HG2 | 23       | 0.15          |
| (3,2412) | 1:10:A:ILE:HA | 1:11:A:GLN:HG2 | 25       | 0.15          |
| (3,2412) | 1:10:A:ILE:HA | 1:11:A:GLN:HG2 | 32       | 0.15          |
| (3,2412) | 1:10:A:ILE:HA | 1:11:A:GLN:HG2 | 37       | 0.15          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,2412) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 39       | 0.15          |
| (3,2412) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 40       | 0.15          |
| (3,2406) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 1        | 0.15          |
| (3,2406) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 1        | 0.15          |
| (3,2406) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 1        | 0.15          |
| (3,2406) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 3        | 0.15          |
| (3,2406) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 3        | 0.15          |
| (3,2406) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 3        | 0.15          |
| (3,2406) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 8        | 0.15          |
| (3,2406) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 8        | 0.15          |
| (3,2406) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 8        | 0.15          |
| (3,2406) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 11       | 0.15          |
| (3,2406) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 11       | 0.15          |
| (3,2406) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 11       | 0.15          |
| (3,2406) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 17       | 0.15          |
| (3,2406) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 17       | 0.15          |
| (3,2406) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 17       | 0.15          |
| (3,2406) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 20       | 0.15          |
| (3,2406) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 20       | 0.15          |
| (3,2406) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 20       | 0.15          |
| (3,2406) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 22       | 0.15          |
| (3,2406) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 22       | 0.15          |
| (3,2406) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 22       | 0.15          |
| (3,2406) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 23       | 0.15          |
| (3,2406) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 23       | 0.15          |
| (3,2406) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 23       | 0.15          |
| (3,2406) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 25       | 0.15          |
| (3,2406) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 25       | 0.15          |
| (3,2406) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 25       | 0.15          |
| (3,2406) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 26       | 0.15          |
| (3,2406) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 26       | 0.15          |
| (3,2406) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 26       | 0.15          |
| (3,2406) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 30       | 0.15          |
| (3,2406) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 30       | 0.15          |
| (3,2406) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 30       | 0.15          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 9        | 0.15          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 9        | 0.15          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 9        | 0.15          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 13       | 0.15          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 13       | 0.15          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 13       | 0.15          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 37       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2405) | 1:66:A:MET:HE2  | 1:29:A:PHE:HZ   | 37       | 0.15          |
| (3,2405) | 1:66:A:MET:HE3  | 1:29:A:PHE:HZ   | 37       | 0.15          |
| (3,2290) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 7        | 0.15          |
| (3,2290) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 12       | 0.15          |
| (3,2290) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 17       | 0.15          |
| (3,2290) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 18       | 0.15          |
| (3,2290) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 22       | 0.15          |
| (3,2290) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 34       | 0.15          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG21 | 8        | 0.15          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG22 | 8        | 0.15          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG23 | 8        | 0.15          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG21 | 20       | 0.15          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG22 | 20       | 0.15          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG23 | 20       | 0.15          |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD11 | 21       | 0.15          |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD12 | 21       | 0.15          |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD13 | 21       | 0.15          |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD11 | 25       | 0.15          |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD12 | 25       | 0.15          |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD13 | 25       | 0.15          |
| (3,2148) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 24       | 0.15          |
| (3,2108) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA   | 28       | 0.15          |
| (3,2108) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA   | 28       | 0.15          |
| (3,2108) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA   | 28       | 0.15          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 4        | 0.15          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 4        | 0.15          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 4        | 0.15          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 21       | 0.15          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 21       | 0.15          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 21       | 0.15          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 22       | 0.15          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 22       | 0.15          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 22       | 0.15          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 25       | 0.15          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 25       | 0.15          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 25       | 0.15          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 30       | 0.15          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 30       | 0.15          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 30       | 0.15          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 38       | 0.15          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 38       | 0.15          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 38       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1  | 3        | 0.15          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2  | 3        | 0.15          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1  | 3        | 0.15          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2  | 3        | 0.15          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1  | 3        | 0.15          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2  | 3        | 0.15          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1  | 9        | 0.15          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2  | 9        | 0.15          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1  | 9        | 0.15          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2  | 9        | 0.15          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1  | 9        | 0.15          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2  | 9        | 0.15          |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD11 | 2        | 0.15          |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD12 | 2        | 0.15          |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD13 | 2        | 0.15          |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD11 | 2        | 0.15          |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD12 | 2        | 0.15          |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD13 | 2        | 0.15          |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD11 | 2        | 0.15          |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD12 | 2        | 0.15          |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD13 | 2        | 0.15          |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD11 | 11       | 0.15          |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD12 | 11       | 0.15          |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD13 | 11       | 0.15          |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD11 | 11       | 0.15          |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD12 | 11       | 0.15          |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD13 | 11       | 0.15          |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD11 | 11       | 0.15          |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD12 | 11       | 0.15          |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD13 | 11       | 0.15          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 5        | 0.15          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 5        | 0.15          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 5        | 0.15          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 13       | 0.15          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 13       | 0.15          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 13       | 0.15          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 30       | 0.15          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 30       | 0.15          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 30       | 0.15          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 36       | 0.15          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 36       | 0.15          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 36       | 0.15          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 15       | 0.15          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 15       | 0.15          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 15       | 0.15          |
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 38       | 0.15          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 38       | 0.15          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 38       | 0.15          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 18       | 0.15          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 18       | 0.15          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 18       | 0.15          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 18       | 0.15          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 18       | 0.15          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 18       | 0.15          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 32       | 0.15          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 32       | 0.15          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 32       | 0.15          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 32       | 0.15          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 32       | 0.15          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 32       | 0.15          |
| (3,2019) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD1 | 18       | 0.15          |
| (3,2019) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD2 | 18       | 0.15          |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1 | 4        | 0.15          |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2 | 4        | 0.15          |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3 | 4        | 0.15          |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1 | 4        | 0.15          |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2 | 4        | 0.15          |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3 | 4        | 0.15          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1 | 4        | 0.15          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2 | 4        | 0.15          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3 | 4        | 0.15          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 9        | 0.15          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 15       | 0.15          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 20       | 0.15          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 23       | 0.15          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 26       | 0.15          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 32       | 0.15          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 34       | 0.15          |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2 | 22       | 0.15          |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2 | 22       | 0.15          |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2 | 22       | 0.15          |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2 | 25       | 0.15          |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2 | 25       | 0.15          |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2 | 25       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1993) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 8        | 0.15          |
| (3,1993) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 8        | 0.15          |
| (3,1993) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 8        | 0.15          |
| (3,1993) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 12       | 0.15          |
| (3,1993) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 12       | 0.15          |
| (3,1993) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 12       | 0.15          |
| (3,1993) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 18       | 0.15          |
| (3,1993) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 18       | 0.15          |
| (3,1993) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 18       | 0.15          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 2        | 0.15          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 7        | 0.15          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 8        | 0.15          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 13       | 0.15          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 22       | 0.15          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 26       | 0.15          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 31       | 0.15          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 32       | 0.15          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 33       | 0.15          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 35       | 0.15          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 38       | 0.15          |
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA   | 6        | 0.15          |
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA   | 6        | 0.15          |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA   | 6        | 0.15          |
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA   | 8        | 0.15          |
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA   | 8        | 0.15          |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA   | 8        | 0.15          |
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA   | 17       | 0.15          |
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA   | 17       | 0.15          |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA   | 17       | 0.15          |
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA   | 20       | 0.15          |
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA   | 20       | 0.15          |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA   | 20       | 0.15          |
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA   | 22       | 0.15          |
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA   | 22       | 0.15          |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA   | 22       | 0.15          |
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA   | 30       | 0.15          |
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA   | 30       | 0.15          |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA   | 30       | 0.15          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H    | 5        | 0.15          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H    | 5        | 0.15          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H    | 5        | 0.15          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H    | 8        | 0.15          |

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| Key      | Atom-1          | Atom-2       | Model ID | Violation (Å) |
|----------|-----------------|--------------|----------|---------------|
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H | 8        | 0.15          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H | 8        | 0.15          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H | 10       | 0.15          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H | 10       | 0.15          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H | 10       | 0.15          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H | 12       | 0.15          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H | 12       | 0.15          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H | 12       | 0.15          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H | 13       | 0.15          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H | 13       | 0.15          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H | 13       | 0.15          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H | 14       | 0.15          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H | 14       | 0.15          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H | 14       | 0.15          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H | 15       | 0.15          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H | 15       | 0.15          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H | 15       | 0.15          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H | 18       | 0.15          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H | 18       | 0.15          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H | 18       | 0.15          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H | 21       | 0.15          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H | 21       | 0.15          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H | 21       | 0.15          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H | 22       | 0.15          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H | 22       | 0.15          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H | 22       | 0.15          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H | 23       | 0.15          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H | 23       | 0.15          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H | 23       | 0.15          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H | 26       | 0.15          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H | 26       | 0.15          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H | 26       | 0.15          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H | 30       | 0.15          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H | 30       | 0.15          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H | 30       | 0.15          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H | 31       | 0.15          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H | 31       | 0.15          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H | 31       | 0.15          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H | 32       | 0.15          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H | 32       | 0.15          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H | 32       | 0.15          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H | 33       | 0.15          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H   | 33       | 0.15          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H   | 33       | 0.15          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H   | 34       | 0.15          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H   | 34       | 0.15          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H   | 34       | 0.15          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H   | 37       | 0.15          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H   | 37       | 0.15          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H   | 37       | 0.15          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H   | 39       | 0.15          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H   | 39       | 0.15          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H   | 39       | 0.15          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H   | 40       | 0.15          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H   | 40       | 0.15          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H   | 40       | 0.15          |
| (3,1866) | 1:7:A:ALA:HB1   | 1:8:A:GLU:H    | 16       | 0.15          |
| (3,1866) | 1:7:A:ALA:HB2   | 1:8:A:GLU:H    | 16       | 0.15          |
| (3,1866) | 1:7:A:ALA:HB3   | 1:8:A:GLU:H    | 16       | 0.15          |
| (3,1864) | 1:7:A:ALA:HB1   | 1:88:A:ARG:HA  | 26       | 0.15          |
| (3,1864) | 1:7:A:ALA:HB2   | 1:88:A:ARG:HA  | 26       | 0.15          |
| (3,1864) | 1:7:A:ALA:HB3   | 1:88:A:ARG:HA  | 26       | 0.15          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 4        | 0.15          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 4        | 0.15          |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 4        | 0.15          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 10       | 0.15          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 10       | 0.15          |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 10       | 0.15          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 14       | 0.15          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 14       | 0.15          |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 14       | 0.15          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 18       | 0.15          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 18       | 0.15          |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 18       | 0.15          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 28       | 0.15          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 28       | 0.15          |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 28       | 0.15          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 34       | 0.15          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 34       | 0.15          |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 34       | 0.15          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 39       | 0.15          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 39       | 0.15          |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 39       | 0.15          |
| (3,1814) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 1        | 0.15          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,1814) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 9        | 0.15          |
| (3,1814) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 12       | 0.15          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 2        | 0.15          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 3        | 0.15          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 11       | 0.15          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 12       | 0.15          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 14       | 0.15          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 16       | 0.15          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 17       | 0.15          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 20       | 0.15          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 24       | 0.15          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 26       | 0.15          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 28       | 0.15          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 33       | 0.15          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 34       | 0.15          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 35       | 0.15          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 37       | 0.15          |
| (3,1781) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H    | 26       | 0.15          |
| (3,1747) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H    | 15       | 0.15          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG11 | 10       | 0.15          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG12 | 10       | 0.15          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG13 | 10       | 0.15          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG11 | 10       | 0.15          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG12 | 10       | 0.15          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG13 | 10       | 0.15          |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG11 | 10       | 0.15          |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG12 | 10       | 0.15          |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG13 | 10       | 0.15          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG11 | 27       | 0.15          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG12 | 27       | 0.15          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG13 | 27       | 0.15          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG11 | 27       | 0.15          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG12 | 27       | 0.15          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG13 | 27       | 0.15          |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG11 | 27       | 0.15          |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG12 | 27       | 0.15          |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG13 | 27       | 0.15          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG11 | 28       | 0.15          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG12 | 28       | 0.15          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG13 | 28       | 0.15          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG11 | 28       | 0.15          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG12 | 28       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 28       | 0.15          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 28       | 0.15          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 28       | 0.15          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 28       | 0.15          |
| (3,1712) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 13       | 0.15          |
| (3,1712) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 13       | 0.15          |
| (3,1712) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 13       | 0.15          |
| (3,1712) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 31       | 0.15          |
| (3,1712) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 31       | 0.15          |
| (3,1712) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 31       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 15       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 15       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 15       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 15       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 15       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 15       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 15       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 15       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 15       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 17       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 17       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 17       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 17       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 17       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 17       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 17       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 17       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 17       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 24       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 24       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 24       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 24       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 24       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 24       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 24       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 24       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 24       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 32       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 32       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 32       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 32       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 32       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 32       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 32       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 32       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 32       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 37       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 37       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 37       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 37       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 37       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 37       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 37       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 37       | 0.15          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 37       | 0.15          |
| (3,1683) | 1:85:A:LEU:HD11 | 1:35:A:PHE:HD1  | 1        | 0.15          |
| (3,1683) | 1:85:A:LEU:HD11 | 1:35:A:PHE:HD2  | 1        | 0.15          |
| (3,1683) | 1:85:A:LEU:HD12 | 1:35:A:PHE:HD1  | 1        | 0.15          |
| (3,1683) | 1:85:A:LEU:HD12 | 1:35:A:PHE:HD2  | 1        | 0.15          |
| (3,1683) | 1:85:A:LEU:HD13 | 1:35:A:PHE:HD1  | 1        | 0.15          |
| (3,1683) | 1:85:A:LEU:HD13 | 1:35:A:PHE:HD2  | 1        | 0.15          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 22       | 0.15          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 22       | 0.15          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 22       | 0.15          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 28       | 0.15          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 28       | 0.15          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 28       | 0.15          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 31       | 0.15          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 31       | 0.15          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 31       | 0.15          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 36       | 0.15          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 36       | 0.15          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 36       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 18       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 18       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 18       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 18       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 18       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 18       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 18       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 18       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 18       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 21       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 21       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 21       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 21       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 21       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 21       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 21       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 21       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 21       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 31       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 31       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 31       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 31       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 31       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 31       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 31       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 31       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 31       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 33       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 33       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 33       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 33       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 33       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 33       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 33       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 33       | 0.15          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 33       | 0.15          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 14       | 0.15          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 14       | 0.15          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 14       | 0.15          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 15       | 0.15          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 15       | 0.15          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 15       | 0.15          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 19       | 0.15          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 19       | 0.15          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 19       | 0.15          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 25       | 0.15          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 25       | 0.15          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 25       | 0.15          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 29       | 0.15          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 29       | 0.15          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 29       | 0.15          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 39       | 0.15          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 39       | 0.15          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 39       | 0.15          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H   | 40       | 0.15          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H   | 40       | 0.15          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 40       | 0.15          |
| (3,1628) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2 | 29       | 0.15          |
| (3,1628) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2 | 29       | 0.15          |
| (3,1628) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2 | 29       | 0.15          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2 | 11       | 0.15          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 11       | 0.15          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 11       | 0.15          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2 | 15       | 0.15          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 15       | 0.15          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 15       | 0.15          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 2        | 0.15          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 2        | 0.15          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 2        | 0.15          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 2        | 0.15          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 2        | 0.15          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 2        | 0.15          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 4        | 0.15          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 4        | 0.15          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 4        | 0.15          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 4        | 0.15          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 4        | 0.15          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 4        | 0.15          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 31       | 0.15          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 31       | 0.15          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 31       | 0.15          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 31       | 0.15          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 31       | 0.15          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 31       | 0.15          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 32       | 0.15          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 32       | 0.15          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 32       | 0.15          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 32       | 0.15          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 32       | 0.15          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 32       | 0.15          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 34       | 0.15          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 34       | 0.15          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 34       | 0.15          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 34       | 0.15          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 34       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2  | 34       | 0.15          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1  | 36       | 0.15          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2  | 36       | 0.15          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1  | 36       | 0.15          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2  | 36       | 0.15          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1  | 36       | 0.15          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2  | 36       | 0.15          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1  | 37       | 0.15          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2  | 37       | 0.15          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1  | 37       | 0.15          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2  | 37       | 0.15          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1  | 37       | 0.15          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2  | 37       | 0.15          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 7        | 0.15          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 7        | 0.15          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 7        | 0.15          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 7        | 0.15          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 7        | 0.15          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 7        | 0.15          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 11       | 0.15          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 11       | 0.15          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 11       | 0.15          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 11       | 0.15          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 11       | 0.15          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 11       | 0.15          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 26       | 0.15          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 26       | 0.15          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 26       | 0.15          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 26       | 0.15          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 26       | 0.15          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 26       | 0.15          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 28       | 0.15          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 28       | 0.15          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 28       | 0.15          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 28       | 0.15          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 28       | 0.15          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 28       | 0.15          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 4        | 0.15          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 4        | 0.15          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 4        | 0.15          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 12       | 0.15          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 12       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 12       | 0.15          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 14       | 0.15          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 14       | 0.15          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 14       | 0.15          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 21       | 0.15          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 21       | 0.15          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 21       | 0.15          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 30       | 0.15          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 30       | 0.15          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 30       | 0.15          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 40       | 0.15          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 40       | 0.15          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 40       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 6        | 0.15          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 6        | 0.15          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 6        | 0.15          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 10       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 10       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 10       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 11       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 11       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 11       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 13       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 13       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 13       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 14       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 14       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 14       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 15       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 15       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 15       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 22       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 22       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 22       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 26       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 26       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 26       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 30       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 30       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 30       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 34       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 34       | 0.15          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA | 34       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA | 37       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA | 37       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA | 37       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA | 40       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA | 40       | 0.15          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA | 40       | 0.15          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H  | 4        | 0.15          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H  | 4        | 0.15          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H  | 4        | 0.15          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H  | 3        | 0.15          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H  | 3        | 0.15          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H  | 3        | 0.15          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H  | 4        | 0.15          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H  | 4        | 0.15          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H  | 4        | 0.15          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H  | 5        | 0.15          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H  | 5        | 0.15          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H  | 5        | 0.15          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H  | 8        | 0.15          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H  | 8        | 0.15          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H  | 8        | 0.15          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H  | 9        | 0.15          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H  | 9        | 0.15          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H  | 9        | 0.15          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H  | 15       | 0.15          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H  | 15       | 0.15          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H  | 15       | 0.15          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H  | 16       | 0.15          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H  | 16       | 0.15          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H  | 16       | 0.15          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H  | 17       | 0.15          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H  | 17       | 0.15          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H  | 17       | 0.15          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H  | 20       | 0.15          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H  | 20       | 0.15          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H  | 20       | 0.15          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H  | 32       | 0.15          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H  | 32       | 0.15          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H  | 32       | 0.15          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H  | 34       | 0.15          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H  | 34       | 0.15          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,1518) | 1:66:A:MET:HE3 | 1:66:A:MET:H   | 34       | 0.15          |
| (3,1518) | 1:66:A:MET:HE1 | 1:66:A:MET:H   | 35       | 0.15          |
| (3,1518) | 1:66:A:MET:HE2 | 1:66:A:MET:H   | 35       | 0.15          |
| (3,1518) | 1:66:A:MET:HE3 | 1:66:A:MET:H   | 35       | 0.15          |
| (3,1518) | 1:66:A:MET:HE1 | 1:66:A:MET:H   | 37       | 0.15          |
| (3,1518) | 1:66:A:MET:HE2 | 1:66:A:MET:H   | 37       | 0.15          |
| (3,1518) | 1:66:A:MET:HE3 | 1:66:A:MET:H   | 37       | 0.15          |
| (3,1517) | 1:66:A:MET:HE1 | 1:29:A:PHE:H   | 13       | 0.15          |
| (3,1517) | 1:66:A:MET:HE2 | 1:29:A:PHE:H   | 13       | 0.15          |
| (3,1517) | 1:66:A:MET:HE3 | 1:29:A:PHE:H   | 13       | 0.15          |
| (3,1517) | 1:66:A:MET:HE1 | 1:29:A:PHE:H   | 20       | 0.15          |
| (3,1517) | 1:66:A:MET:HE2 | 1:29:A:PHE:H   | 20       | 0.15          |
| (3,1517) | 1:66:A:MET:HE3 | 1:29:A:PHE:H   | 20       | 0.15          |
| (3,1514) | 1:66:A:MET:HE1 | 1:42:A:TRP:HE1 | 15       | 0.15          |
| (3,1514) | 1:66:A:MET:HE2 | 1:42:A:TRP:HE1 | 15       | 0.15          |
| (3,1514) | 1:66:A:MET:HE3 | 1:42:A:TRP:HE1 | 15       | 0.15          |
| (3,1514) | 1:66:A:MET:HE1 | 1:42:A:TRP:HE1 | 19       | 0.15          |
| (3,1514) | 1:66:A:MET:HE2 | 1:42:A:TRP:HE1 | 19       | 0.15          |
| (3,1514) | 1:66:A:MET:HE3 | 1:42:A:TRP:HE1 | 19       | 0.15          |
| (3,1514) | 1:66:A:MET:HE1 | 1:42:A:TRP:HE1 | 21       | 0.15          |
| (3,1514) | 1:66:A:MET:HE2 | 1:42:A:TRP:HE1 | 21       | 0.15          |
| (3,1514) | 1:66:A:MET:HE3 | 1:42:A:TRP:HE1 | 21       | 0.15          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 19       | 0.15          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 19       | 0.15          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 19       | 0.15          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 19       | 0.15          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 19       | 0.15          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 19       | 0.15          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 27       | 0.15          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 27       | 0.15          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 27       | 0.15          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 27       | 0.15          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 27       | 0.15          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 27       | 0.15          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 33       | 0.15          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 33       | 0.15          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 33       | 0.15          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 33       | 0.15          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 33       | 0.15          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 33       | 0.15          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 35       | 0.15          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 35       | 0.15          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1 | 35       | 0.15          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2 | 35       | 0.15          |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE1 | 35       | 0.15          |
| (3,1513) | 1:66:A:MET:HE3  | 1:79:A:TYR:HE2 | 35       | 0.15          |
| (3,1512) | 1:66:A:MET:HE1  | 1:42:A:TRP:HZ3 | 20       | 0.15          |
| (3,1512) | 1:66:A:MET:HE2  | 1:42:A:TRP:HZ3 | 20       | 0.15          |
| (3,1512) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3 | 20       | 0.15          |
| (3,1512) | 1:66:A:MET:HE1  | 1:42:A:TRP:HZ3 | 23       | 0.15          |
| (3,1512) | 1:66:A:MET:HE2  | 1:42:A:TRP:HZ3 | 23       | 0.15          |
| (3,1512) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3 | 23       | 0.15          |
| (3,1512) | 1:66:A:MET:HE1  | 1:42:A:TRP:HZ3 | 25       | 0.15          |
| (3,1512) | 1:66:A:MET:HE2  | 1:42:A:TRP:HZ3 | 25       | 0.15          |
| (3,1512) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3 | 25       | 0.15          |
| (3,1512) | 1:66:A:MET:HE1  | 1:42:A:TRP:HZ3 | 27       | 0.15          |
| (3,1512) | 1:66:A:MET:HE2  | 1:42:A:TRP:HZ3 | 27       | 0.15          |
| (3,1512) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3 | 27       | 0.15          |
| (3,1512) | 1:66:A:MET:HE1  | 1:42:A:TRP:HZ3 | 38       | 0.15          |
| (3,1512) | 1:66:A:MET:HE2  | 1:42:A:TRP:HZ3 | 38       | 0.15          |
| (3,1512) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3 | 38       | 0.15          |
| (3,1504) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2 | 2        | 0.15          |
| (3,1504) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2 | 2        | 0.15          |
| (3,1504) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2 | 2        | 0.15          |
| (3,1504) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2 | 7        | 0.15          |
| (3,1504) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2 | 7        | 0.15          |
| (3,1504) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2 | 7        | 0.15          |
| (3,1504) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2 | 10       | 0.15          |
| (3,1504) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2 | 10       | 0.15          |
| (3,1504) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2 | 10       | 0.15          |
| (3,1504) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2 | 21       | 0.15          |
| (3,1504) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2 | 21       | 0.15          |
| (3,1504) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2 | 21       | 0.15          |
| (3,1504) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2 | 28       | 0.15          |
| (3,1504) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2 | 28       | 0.15          |
| (3,1504) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2 | 28       | 0.15          |
| (3,1498) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ  | 20       | 0.15          |
| (3,1498) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ  | 20       | 0.15          |
| (3,1498) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ  | 20       | 0.15          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 16       | 0.15          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 16       | 0.15          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 16       | 0.15          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 27       | 0.15          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 27       | 0.15          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 27       | 0.15          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H   | 5        | 0.15          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H   | 5        | 0.15          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H   | 5        | 0.15          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H   | 20       | 0.15          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H   | 20       | 0.15          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H   | 20       | 0.15          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H   | 28       | 0.15          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H   | 28       | 0.15          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H   | 28       | 0.15          |
| (3,1470) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 26       | 0.15          |
| (3,1470) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 26       | 0.15          |
| (3,1470) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 26       | 0.15          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 17       | 0.15          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 17       | 0.15          |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 17       | 0.15          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 29       | 0.15          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 29       | 0.15          |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 29       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H   | 11       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H   | 11       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H   | 11       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H   | 13       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H   | 13       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H   | 13       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H   | 15       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H   | 15       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H   | 15       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H   | 18       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H   | 18       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H   | 18       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H   | 19       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H   | 19       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H   | 19       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H   | 23       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H   | 23       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H   | 23       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H   | 33       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H   | 33       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H   | 33       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H   | 35       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H   | 35       | 0.15          |

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| Key      | Atom-1         | Atom-2       | Model ID | Violation (Å) |
|----------|----------------|--------------|----------|---------------|
| (3,1407) | 1:95:A:ALA:HB3 | 1:18:A:ASN:H | 35       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB1 | 1:18:A:ASN:H | 36       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB2 | 1:18:A:ASN:H | 36       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB3 | 1:18:A:ASN:H | 36       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB1 | 1:18:A:ASN:H | 38       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB2 | 1:18:A:ASN:H | 38       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB3 | 1:18:A:ASN:H | 38       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB1 | 1:18:A:ASN:H | 40       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB2 | 1:18:A:ASN:H | 40       | 0.15          |
| (3,1407) | 1:95:A:ALA:HB3 | 1:18:A:ASN:H | 40       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H | 1        | 0.15          |
| (3,1405) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H | 1        | 0.15          |
| (3,1405) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H | 1        | 0.15          |
| (3,1405) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H | 4        | 0.15          |
| (3,1405) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H | 4        | 0.15          |
| (3,1405) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H | 4        | 0.15          |
| (3,1405) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H | 8        | 0.15          |
| (3,1405) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H | 8        | 0.15          |
| (3,1405) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H | 8        | 0.15          |
| (3,1405) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H | 10       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H | 10       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H | 10       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H | 12       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H | 12       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H | 12       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H | 16       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H | 16       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H | 16       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H | 18       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H | 18       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H | 18       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H | 20       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H | 20       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H | 20       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H | 23       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H | 23       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H | 23       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H | 24       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H | 24       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H | 24       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H | 25       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H | 25       | 0.15          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,1405) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 25       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H    | 30       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H    | 30       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 30       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H    | 32       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H    | 32       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 32       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H    | 34       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H    | 34       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 34       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H    | 35       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H    | 35       | 0.15          |
| (3,1405) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 35       | 0.15          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 1        | 0.15          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 1        | 0.15          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 1        | 0.15          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 9        | 0.15          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 9        | 0.15          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 9        | 0.15          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 12       | 0.15          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 12       | 0.15          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 12       | 0.15          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 23       | 0.15          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 23       | 0.15          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 23       | 0.15          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 29       | 0.15          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 29       | 0.15          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 29       | 0.15          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 36       | 0.15          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 36       | 0.15          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 36       | 0.15          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 37       | 0.15          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 37       | 0.15          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 37       | 0.15          |
| (3,1391) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ   | 9        | 0.15          |
| (3,1391) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ   | 9        | 0.15          |
| (3,1391) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ   | 9        | 0.15          |
| (3,1391) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ   | 15       | 0.15          |
| (3,1391) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ   | 15       | 0.15          |
| (3,1391) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ   | 15       | 0.15          |
| (3,1391) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ   | 33       | 0.15          |
| (3,1391) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ   | 33       | 0.15          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,1391) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ  | 33       | 0.15          |
| (3,1391) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ  | 34       | 0.15          |
| (3,1391) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ  | 34       | 0.15          |
| (3,1391) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ  | 34       | 0.15          |
| (3,1391) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ  | 37       | 0.15          |
| (3,1391) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ  | 37       | 0.15          |
| (3,1391) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ  | 37       | 0.15          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 26       | 0.15          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 26       | 0.15          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 26       | 0.15          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 26       | 0.15          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 26       | 0.15          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 26       | 0.15          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 26       | 0.15          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 26       | 0.15          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 26       | 0.15          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 37       | 0.15          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 37       | 0.15          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 37       | 0.15          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 37       | 0.15          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 37       | 0.15          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 37       | 0.15          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 37       | 0.15          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 37       | 0.15          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 37       | 0.15          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 38       | 0.15          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 38       | 0.15          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 38       | 0.15          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 38       | 0.15          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 38       | 0.15          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 38       | 0.15          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 38       | 0.15          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 38       | 0.15          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 38       | 0.15          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 26       | 0.15          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 26       | 0.15          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 26       | 0.15          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 26       | 0.15          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 26       | 0.15          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 26       | 0.15          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 26       | 0.15          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 26       | 0.15          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3  | 26       | 0.15          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1  | 37       | 0.15          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2  | 37       | 0.15          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3  | 37       | 0.15          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1  | 37       | 0.15          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2  | 37       | 0.15          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3  | 37       | 0.15          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1  | 37       | 0.15          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2  | 37       | 0.15          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3  | 37       | 0.15          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1  | 38       | 0.15          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2  | 38       | 0.15          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3  | 38       | 0.15          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1  | 38       | 0.15          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2  | 38       | 0.15          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3  | 38       | 0.15          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1  | 38       | 0.15          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2  | 38       | 0.15          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3  | 38       | 0.15          |
| (3,1372) | 1:16:A:ILE:HB  | 1:29:A:PHE:HB3  | 3        | 0.15          |
| (3,1372) | 1:16:A:ILE:HB  | 1:29:A:PHE:HB3  | 19       | 0.15          |
| (3,1372) | 1:16:A:ILE:HB  | 1:29:A:PHE:HB3  | 21       | 0.15          |
| (3,1372) | 1:16:A:ILE:HB  | 1:29:A:PHE:HB3  | 32       | 0.15          |
| (3,1329) | 1:19:A:ILE:HB  | 1:20:A:VAL:H    | 2        | 0.15          |
| (3,1329) | 1:19:A:ILE:HB  | 1:20:A:VAL:H    | 16       | 0.15          |
| (3,1329) | 1:19:A:ILE:HB  | 1:20:A:VAL:H    | 17       | 0.15          |
| (3,1329) | 1:19:A:ILE:HB  | 1:20:A:VAL:H    | 22       | 0.15          |
| (3,1329) | 1:19:A:ILE:HB  | 1:20:A:VAL:H    | 28       | 0.15          |
| (3,1299) | 1:40:A:VAL:HB  | 1:41:A:THR:H    | 1        | 0.15          |
| (3,1299) | 1:40:A:VAL:HB  | 1:41:A:THR:H    | 24       | 0.15          |
| (3,1295) | 1:40:A:VAL:HB  | 1:81:A:VAL:HG21 | 1        | 0.15          |
| (3,1295) | 1:40:A:VAL:HB  | 1:81:A:VAL:HG22 | 1        | 0.15          |
| (3,1295) | 1:40:A:VAL:HB  | 1:81:A:VAL:HG23 | 1        | 0.15          |
| (3,1295) | 1:40:A:VAL:HB  | 1:81:A:VAL:HG21 | 4        | 0.15          |
| (3,1295) | 1:40:A:VAL:HB  | 1:81:A:VAL:HG22 | 4        | 0.15          |
| (3,1295) | 1:40:A:VAL:HB  | 1:81:A:VAL:HG23 | 4        | 0.15          |
| (3,1295) | 1:40:A:VAL:HB  | 1:81:A:VAL:HG21 | 6        | 0.15          |
| (3,1295) | 1:40:A:VAL:HB  | 1:81:A:VAL:HG22 | 6        | 0.15          |
| (3,1295) | 1:40:A:VAL:HB  | 1:81:A:VAL:HG23 | 6        | 0.15          |
| (3,1295) | 1:40:A:VAL:HB  | 1:81:A:VAL:HG21 | 10       | 0.15          |
| (3,1295) | 1:40:A:VAL:HB  | 1:81:A:VAL:HG22 | 10       | 0.15          |
| (3,1295) | 1:40:A:VAL:HB  | 1:81:A:VAL:HG23 | 10       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 13       | 0.15          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 13       | 0.15          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 13       | 0.15          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 23       | 0.15          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 23       | 0.15          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 23       | 0.15          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 27       | 0.15          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 27       | 0.15          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 27       | 0.15          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 34       | 0.15          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 34       | 0.15          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 34       | 0.15          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 39       | 0.15          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 39       | 0.15          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 39       | 0.15          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1  | 4        | 0.15          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2  | 4        | 0.15          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3  | 4        | 0.15          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1  | 4        | 0.15          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2  | 4        | 0.15          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3  | 4        | 0.15          |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1  | 4        | 0.15          |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2  | 4        | 0.15          |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3  | 4        | 0.15          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 1        | 0.15          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 1        | 0.15          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 1        | 0.15          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 4        | 0.15          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 4        | 0.15          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 4        | 0.15          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 6        | 0.15          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 6        | 0.15          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 6        | 0.15          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 10       | 0.15          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 10       | 0.15          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 10       | 0.15          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 13       | 0.15          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 13       | 0.15          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 13       | 0.15          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 23       | 0.15          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 23       | 0.15          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 23       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 27       | 0.15          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 27       | 0.15          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 27       | 0.15          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 34       | 0.15          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 34       | 0.15          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 34       | 0.15          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 39       | 0.15          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 39       | 0.15          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 39       | 0.15          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 5        | 0.15          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 5        | 0.15          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 5        | 0.15          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 5        | 0.15          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 5        | 0.15          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 5        | 0.15          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 5        | 0.15          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 5        | 0.15          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 5        | 0.15          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 6        | 0.15          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 6        | 0.15          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 6        | 0.15          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 6        | 0.15          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 6        | 0.15          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 6        | 0.15          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 6        | 0.15          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 6        | 0.15          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 6        | 0.15          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 7        | 0.15          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 7        | 0.15          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 7        | 0.15          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 7        | 0.15          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 7        | 0.15          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 7        | 0.15          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 7        | 0.15          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 7        | 0.15          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 7        | 0.15          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 9        | 0.15          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 9        | 0.15          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 9        | 0.15          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 9        | 0.15          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 9        | 0.15          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 9        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 9        | 0.15          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 9        | 0.15          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 9        | 0.15          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 11       | 0.15          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 11       | 0.15          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 11       | 0.15          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 11       | 0.15          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 11       | 0.15          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 11       | 0.15          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 11       | 0.15          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 11       | 0.15          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 11       | 0.15          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 25       | 0.15          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 25       | 0.15          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 25       | 0.15          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 25       | 0.15          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 25       | 0.15          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 25       | 0.15          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 25       | 0.15          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 25       | 0.15          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 25       | 0.15          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 31       | 0.15          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 31       | 0.15          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 31       | 0.15          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 31       | 0.15          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 31       | 0.15          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 31       | 0.15          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 31       | 0.15          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 31       | 0.15          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 31       | 0.15          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 36       | 0.15          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 36       | 0.15          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 36       | 0.15          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 36       | 0.15          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 36       | 0.15          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 36       | 0.15          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 36       | 0.15          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 36       | 0.15          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 36       | 0.15          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 7        | 0.15          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 7        | 0.15          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 7        | 0.15          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA  | 14       | 0.15          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA  | 14       | 0.15          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA  | 14       | 0.15          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA  | 19       | 0.15          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA  | 19       | 0.15          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA  | 19       | 0.15          |
| (3,1261) | 1:67:A:THR:HG21 | 1:26:A:SER:HB2 | 11       | 0.15          |
| (3,1261) | 1:67:A:THR:HG22 | 1:26:A:SER:HB2 | 11       | 0.15          |
| (3,1261) | 1:67:A:THR:HG23 | 1:26:A:SER:HB2 | 11       | 0.15          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H   | 2        | 0.15          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H   | 2        | 0.15          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H   | 2        | 0.15          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H   | 6        | 0.15          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H   | 6        | 0.15          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H   | 6        | 0.15          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H   | 9        | 0.15          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H   | 9        | 0.15          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H   | 9        | 0.15          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H   | 18       | 0.15          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H   | 18       | 0.15          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H   | 18       | 0.15          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H   | 23       | 0.15          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H   | 23       | 0.15          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H   | 23       | 0.15          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H   | 29       | 0.15          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H   | 29       | 0.15          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H   | 29       | 0.15          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H   | 30       | 0.15          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H   | 30       | 0.15          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H   | 30       | 0.15          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H   | 32       | 0.15          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H   | 32       | 0.15          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H   | 32       | 0.15          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H   | 38       | 0.15          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H   | 38       | 0.15          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H   | 38       | 0.15          |
| (3,1243) | 1:13:A:THR:HG21 | 1:34:A:SER:H   | 14       | 0.15          |
| (3,1243) | 1:13:A:THR:HG22 | 1:34:A:SER:H   | 14       | 0.15          |
| (3,1243) | 1:13:A:THR:HG23 | 1:34:A:SER:H   | 14       | 0.15          |
| (3,1243) | 1:13:A:THR:HG21 | 1:34:A:SER:H   | 23       | 0.15          |
| (3,1243) | 1:13:A:THR:HG22 | 1:34:A:SER:H   | 23       | 0.15          |
| (3,1243) | 1:13:A:THR:HG23 | 1:34:A:SER:H   | 23       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1243) | 1:13:A:THR:HG21 | 1:34:A:SER:H    | 36       | 0.15          |
| (3,1243) | 1:13:A:THR:HG22 | 1:34:A:SER:H    | 36       | 0.15          |
| (3,1243) | 1:13:A:THR:HG23 | 1:34:A:SER:H    | 36       | 0.15          |
| (3,1230) | 1:101:A:LEU:H   | 1:22:A:SER:HA   | 15       | 0.15          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 15       | 0.15          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 15       | 0.15          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 15       | 0.15          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 27       | 0.15          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 27       | 0.15          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 27       | 0.15          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 24       | 0.15          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 24       | 0.15          |
| (3,1204) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 24       | 0.15          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 4        | 0.15          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 4        | 0.15          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 4        | 0.15          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 10       | 0.15          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 10       | 0.15          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 10       | 0.15          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 11       | 0.15          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 11       | 0.15          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 11       | 0.15          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 14       | 0.15          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 14       | 0.15          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 14       | 0.15          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 16       | 0.15          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 16       | 0.15          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 16       | 0.15          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 17       | 0.15          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 17       | 0.15          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 17       | 0.15          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 22       | 0.15          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 22       | 0.15          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 22       | 0.15          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 40       | 0.15          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 40       | 0.15          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 40       | 0.15          |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 5        | 0.15          |
| (3,1181) | 1:100:A:GLU:H   | 1:21:A:VAL:HG11 | 6        | 0.15          |
| (3,1181) | 1:100:A:GLU:H   | 1:21:A:VAL:HG12 | 6        | 0.15          |
| (3,1181) | 1:100:A:GLU:H   | 1:21:A:VAL:HG13 | 6        | 0.15          |
| (3,1178) | 1:91:A:ALA:H    | 1:84:A:ARG:HA   | 5        | 0.15          |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (3,1167) | 1:75:A:ASP:H  | 1:74:A:ASP:HB2  | 11       | 0.15          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 7        | 0.15          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 7        | 0.15          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 9        | 0.15          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 9        | 0.15          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 18       | 0.15          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 18       | 0.15          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 26       | 0.15          |
| (3,1166) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 26       | 0.15          |
| (3,1140) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 6        | 0.15          |
| (3,1096) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 22       | 0.15          |
| (3,1051) | 1:26:A:SER:H  | 1:25:A:GLN:HG2  | 20       | 0.15          |
| (3,1051) | 1:26:A:SER:H  | 1:25:A:GLN:HG2  | 29       | 0.15          |
| (3,1019) | 1:48:A:GLU:H  | 1:48:A:GLU:HG3  | 6        | 0.15          |
| (3,1019) | 1:48:A:GLU:H  | 1:48:A:GLU:HG3  | 11       | 0.15          |
| (3,1019) | 1:48:A:GLU:H  | 1:48:A:GLU:HG3  | 29       | 0.15          |
| (3,1003) | 1:5:A:PHE:H   | 1:4:A:PRO:HA    | 15       | 0.15          |
| (3,1003) | 1:5:A:PHE:H   | 1:4:A:PRO:HA    | 18       | 0.15          |
| (3,998)  | 1:79:A:TYR:H  | 1:94:A:THR:HG21 | 2        | 0.15          |
| (3,998)  | 1:79:A:TYR:H  | 1:94:A:THR:HG22 | 2        | 0.15          |
| (3,998)  | 1:79:A:TYR:H  | 1:94:A:THR:HG23 | 2        | 0.15          |
| (3,998)  | 1:79:A:TYR:H  | 1:94:A:THR:HG21 | 19       | 0.15          |
| (3,998)  | 1:79:A:TYR:H  | 1:94:A:THR:HG22 | 19       | 0.15          |
| (3,998)  | 1:79:A:TYR:H  | 1:94:A:THR:HG23 | 19       | 0.15          |
| (3,988)  | 1:12:A:PHE:H  | 1:11:A:GLN:HB2  | 16       | 0.15          |
| (3,988)  | 1:12:A:PHE:H  | 1:11:A:GLN:HB2  | 18       | 0.15          |
| (3,988)  | 1:12:A:PHE:H  | 1:11:A:GLN:HB2  | 22       | 0.15          |
| (3,988)  | 1:12:A:PHE:H  | 1:11:A:GLN:HB2  | 24       | 0.15          |
| (3,988)  | 1:12:A:PHE:H  | 1:11:A:GLN:HB2  | 25       | 0.15          |
| (3,988)  | 1:12:A:PHE:H  | 1:11:A:GLN:HB2  | 28       | 0.15          |
| (3,988)  | 1:12:A:PHE:H  | 1:11:A:GLN:HB2  | 30       | 0.15          |
| (3,988)  | 1:12:A:PHE:H  | 1:11:A:GLN:HB2  | 32       | 0.15          |
| (3,988)  | 1:12:A:PHE:H  | 1:11:A:GLN:HB2  | 35       | 0.15          |
| (3,988)  | 1:12:A:PHE:H  | 1:11:A:GLN:HB2  | 37       | 0.15          |
| (3,988)  | 1:12:A:PHE:H  | 1:11:A:GLN:HB2  | 40       | 0.15          |
| (3,979)  | 1:20:A:VAL:H  | 1:19:A:ILE:HB   | 2        | 0.15          |
| (3,979)  | 1:20:A:VAL:H  | 1:19:A:ILE:HB   | 16       | 0.15          |
| (3,979)  | 1:20:A:VAL:H  | 1:19:A:ILE:HB   | 17       | 0.15          |
| (3,979)  | 1:20:A:VAL:H  | 1:19:A:ILE:HB   | 22       | 0.15          |
| (3,979)  | 1:20:A:VAL:H  | 1:19:A:ILE:HB   | 28       | 0.15          |
| (3,972)  | 1:21:A:VAL:H  | 1:21:A:VAL:HG21 | 5        | 0.15          |
| (3,972)  | 1:21:A:VAL:H  | 1:21:A:VAL:HG22 | 5        | 0.15          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,972) | 1:21:A:VAL:H | 1:21:A:VAL:HG23 | 5        | 0.15          |
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 3        | 0.15          |
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 12       | 0.15          |
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 18       | 0.15          |
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 29       | 0.15          |
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 37       | 0.15          |
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 38       | 0.15          |
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 39       | 0.15          |
| (3,942) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 3        | 0.15          |
| (3,942) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 31       | 0.15          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 2        | 0.15          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 2        | 0.15          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 2        | 0.15          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 4        | 0.15          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 4        | 0.15          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 4        | 0.15          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 10       | 0.15          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 10       | 0.15          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 10       | 0.15          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 12       | 0.15          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 12       | 0.15          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 12       | 0.15          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 15       | 0.15          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 15       | 0.15          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 15       | 0.15          |
| (3,900) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 20       | 0.15          |
| (3,889) | 1:80:A:SER:H | 1:43:A:TYR:HB3  | 1        | 0.15          |
| (3,889) | 1:80:A:SER:H | 1:43:A:TYR:HB3  | 5        | 0.15          |
| (3,889) | 1:80:A:SER:H | 1:43:A:TYR:HB3  | 30       | 0.15          |
| (3,875) | 1:8:A:GLU:H  | 1:7:A:ALA:HB1   | 16       | 0.15          |
| (3,875) | 1:8:A:GLU:H  | 1:7:A:ALA:HB2   | 16       | 0.15          |
| (3,875) | 1:8:A:GLU:H  | 1:7:A:ALA:HB3   | 16       | 0.15          |
| (3,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3   | 2        | 0.15          |
| (3,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3   | 8        | 0.15          |
| (3,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 22       | 0.15          |
| (3,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 35       | 0.15          |
| (3,863) | 1:86:A:GLU:H | 1:85:A:LEU:HB3  | 33       | 0.15          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 22       | 0.15          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 22       | 0.15          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 22       | 0.15          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 30       | 0.15          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 30       | 0.15          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (3,849) | 1:83:A:ALA:H  | 1:91:A:ALA:HB3  | 30       | 0.15          |
| (3,849) | 1:83:A:ALA:H  | 1:91:A:ALA:HB1  | 32       | 0.15          |
| (3,849) | 1:83:A:ALA:H  | 1:91:A:ALA:HB2  | 32       | 0.15          |
| (3,849) | 1:83:A:ALA:H  | 1:91:A:ALA:HB3  | 32       | 0.15          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG21 | 5        | 0.15          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG22 | 5        | 0.15          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG23 | 5        | 0.15          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG21 | 29       | 0.15          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG22 | 29       | 0.15          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG23 | 29       | 0.15          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG21 | 39       | 0.15          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG22 | 39       | 0.15          |
| (3,814) | 1:25:A:GLN:H  | 1:71:A:VAL:HG23 | 39       | 0.15          |
| (3,810) | 1:25:A:GLN:H  | 1:71:A:VAL:HB   | 20       | 0.15          |
| (3,810) | 1:25:A:GLN:H  | 1:71:A:VAL:HB   | 22       | 0.15          |
| (3,810) | 1:25:A:GLN:H  | 1:71:A:VAL:HB   | 23       | 0.15          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG11 | 5        | 0.15          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG12 | 5        | 0.15          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG13 | 5        | 0.15          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG11 | 20       | 0.15          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG12 | 20       | 0.15          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG13 | 20       | 0.15          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG11 | 28       | 0.15          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG12 | 28       | 0.15          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG13 | 28       | 0.15          |
| (3,801) | 1:54:A:LYS:H  | 1:54:A:LYS:HD2  | 19       | 0.15          |
| (3,801) | 1:54:A:LYS:H  | 1:54:A:LYS:HD2  | 28       | 0.15          |
| (3,786) | 1:6:A:THR:H   | 1:6:A:THR:HG21  | 29       | 0.15          |
| (3,786) | 1:6:A:THR:H   | 1:6:A:THR:HG22  | 29       | 0.15          |
| (3,786) | 1:6:A:THR:H   | 1:6:A:THR:HG23  | 29       | 0.15          |
| (3,776) | 1:6:A:THR:H   | 1:6:A:THR:HA    | 16       | 0.15          |
| (3,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 22       | 0.15          |
| (3,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 27       | 0.15          |
| (3,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 30       | 0.15          |
| (3,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 38       | 0.15          |
| (3,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 7        | 0.15          |
| (3,672) | 1:72:A:THR:H  | 1:73:A:PRO:HD2  | 18       | 0.15          |
| (3,661) | 1:7:A:ALA:H   | 1:6:A:THR:HA    | 8        | 0.15          |
| (3,661) | 1:7:A:ALA:H   | 1:6:A:THR:HA    | 23       | 0.15          |
| (3,661) | 1:7:A:ALA:H   | 1:6:A:THR:HA    | 36       | 0.15          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 9        | 0.15          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 16       | 0.15          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 24       | 0.15          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 34       | 0.15          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 39       | 0.15          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 40       | 0.15          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 24       | 0.15          |
| (3,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 37       | 0.15          |
| (3,591) | 1:3:A:ASP:H   | 1:3:A:ASP:HA    | 40       | 0.15          |
| (3,589) | 1:93:A:SER:H  | 1:92:A:ARG:HG2  | 3        | 0.15          |
| (3,589) | 1:93:A:SER:H  | 1:92:A:ARG:HG2  | 12       | 0.15          |
| (3,589) | 1:93:A:SER:H  | 1:92:A:ARG:HG2  | 23       | 0.15          |
| (3,589) | 1:93:A:SER:H  | 1:92:A:ARG:HG2  | 28       | 0.15          |
| (3,589) | 1:93:A:SER:H  | 1:92:A:ARG:HG2  | 35       | 0.15          |
| (3,589) | 1:93:A:SER:H  | 1:92:A:ARG:HG2  | 38       | 0.15          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 2        | 0.15          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 2        | 0.15          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 2        | 0.15          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 11       | 0.15          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 11       | 0.15          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 11       | 0.15          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 21       | 0.15          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 21       | 0.15          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 21       | 0.15          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 22       | 0.15          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 22       | 0.15          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 22       | 0.15          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 23       | 0.15          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 23       | 0.15          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 23       | 0.15          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 25       | 0.15          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 25       | 0.15          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 25       | 0.15          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 30       | 0.15          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 30       | 0.15          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 30       | 0.15          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 34       | 0.15          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 34       | 0.15          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 34       | 0.15          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 36       | 0.15          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 36       | 0.15          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 36       | 0.15          |
| (3,560) | 1:47:A:THR:H  | 1:47:A:THR:HA   | 18       | 0.15          |
| (3,560) | 1:47:A:THR:H  | 1:47:A:THR:HA   | 19       | 0.15          |

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| Key     | Atom-1       | Atom-2         | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (3,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 31       | 0.15          |
| (3,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 33       | 0.15          |
| (3,560) | 1:47:A:THR:H | 1:47:A:THR:HA  | 39       | 0.15          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1 | 7        | 0.15          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2 | 7        | 0.15          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1 | 19       | 0.15          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2 | 19       | 0.15          |
| (3,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2 | 8        | 0.15          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 6        | 0.15          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 12       | 0.15          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 14       | 0.15          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2 | 37       | 0.15          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2 | 13       | 0.15          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2 | 29       | 0.15          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2 | 31       | 0.15          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2 | 3        | 0.15          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2 | 4        | 0.15          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2 | 6        | 0.15          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2 | 11       | 0.15          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2 | 13       | 0.15          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2 | 19       | 0.15          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2 | 21       | 0.15          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2 | 23       | 0.15          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2 | 25       | 0.15          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2 | 31       | 0.15          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2 | 33       | 0.15          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2 | 35       | 0.15          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2 | 36       | 0.15          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2 | 37       | 0.15          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2 | 39       | 0.15          |
| (3,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3 | 5        | 0.15          |
| (3,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3 | 8        | 0.15          |
| (3,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3 | 15       | 0.15          |
| (3,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3 | 37       | 0.15          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2 | 1        | 0.15          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2 | 2        | 0.15          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2 | 10       | 0.15          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2 | 11       | 0.15          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2 | 18       | 0.15          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2 | 21       | 0.15          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2 | 24       | 0.15          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2 | 31       | 0.15          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 32       | 0.15          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 33       | 0.15          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 34       | 0.15          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 40       | 0.15          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 2        | 0.15          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 5        | 0.15          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 12       | 0.15          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 16       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 3        | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 3        | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 3        | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 4        | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 4        | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 4        | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 9        | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 9        | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 9        | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 11       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 11       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 11       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 15       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 15       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 15       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 16       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 16       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 16       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 20       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 20       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 20       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 22       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 22       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 22       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 23       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 23       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 23       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 25       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 25       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 25       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 26       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 26       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 26       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 28       | 0.15          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 28       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 28       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 32       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 32       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 32       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 36       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 36       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 36       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 37       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 37       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 37       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 38       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 38       | 0.15          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 38       | 0.15          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 11       | 0.15          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 11       | 0.15          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 11       | 0.15          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 13       | 0.15          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 13       | 0.15          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 13       | 0.15          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 15       | 0.15          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 15       | 0.15          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 15       | 0.15          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 18       | 0.15          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 18       | 0.15          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 18       | 0.15          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 19       | 0.15          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 19       | 0.15          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 19       | 0.15          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 23       | 0.15          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 23       | 0.15          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 23       | 0.15          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 33       | 0.15          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 33       | 0.15          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 33       | 0.15          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 35       | 0.15          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 35       | 0.15          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 35       | 0.15          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 36       | 0.15          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 36       | 0.15          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 36       | 0.15          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 38       | 0.15          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (3,370) | 1:18:A:ASN:H  | 1:95:A:ALA:HB2  | 38       | 0.15          |
| (3,370) | 1:18:A:ASN:H  | 1:95:A:ALA:HB3  | 38       | 0.15          |
| (3,370) | 1:18:A:ASN:H  | 1:95:A:ALA:HB1  | 40       | 0.15          |
| (3,370) | 1:18:A:ASN:H  | 1:95:A:ALA:HB2  | 40       | 0.15          |
| (3,370) | 1:18:A:ASN:H  | 1:95:A:ALA:HB3  | 40       | 0.15          |
| (3,368) | 1:18:A:ASN:H  | 1:17:A:GLN:HB3  | 5        | 0.15          |
| (3,343) | 1:14:A:LYS:H  | 1:33:A:VAL:HA   | 20       | 0.15          |
| (3,339) | 1:14:A:LYS:H  | 1:12:A:PHE:HD1  | 12       | 0.15          |
| (3,339) | 1:14:A:LYS:H  | 1:12:A:PHE:HD2  | 12       | 0.15          |
| (3,314) | 1:63:A:CYS:H  | 1:64:A:HIS:HD2  | 27       | 0.15          |
| (3,296) | 1:31:A:CYS:H  | 1:30:A:GLU:HB3  | 9        | 0.15          |
| (3,296) | 1:31:A:CYS:H  | 1:30:A:GLU:HB3  | 15       | 0.15          |
| (3,296) | 1:31:A:CYS:H  | 1:30:A:GLU:HB3  | 20       | 0.15          |
| (3,296) | 1:31:A:CYS:H  | 1:30:A:GLU:HB3  | 23       | 0.15          |
| (3,296) | 1:31:A:CYS:H  | 1:30:A:GLU:HB3  | 26       | 0.15          |
| (3,296) | 1:31:A:CYS:H  | 1:30:A:GLU:HB3  | 32       | 0.15          |
| (3,296) | 1:31:A:CYS:H  | 1:30:A:GLU:HB3  | 34       | 0.15          |
| (3,274) | 1:66:A:MET:H  | 1:66:A:MET:HG3  | 4        | 0.15          |
| (3,242) | 1:95:A:ALA:H  | 1:96:A:GLU:H    | 28       | 0.15          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD1  | 6        | 0.15          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD2  | 6        | 0.15          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD1  | 9        | 0.15          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD2  | 9        | 0.15          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD1  | 20       | 0.15          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD2  | 20       | 0.15          |
| (3,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 3        | 0.15          |
| (3,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 5        | 0.15          |
| (3,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 8        | 0.15          |
| (3,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 10       | 0.15          |
| (3,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 12       | 0.15          |
| (3,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 20       | 0.15          |
| (3,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 27       | 0.15          |
| (3,198) | 1:90:A:GLU:H  | 1:90:A:GLU:HB2  | 27       | 0.15          |
| (3,198) | 1:90:A:GLU:H  | 1:90:A:GLU:HB2  | 28       | 0.15          |
| (3,198) | 1:90:A:GLU:H  | 1:90:A:GLU:HB2  | 30       | 0.15          |
| (3,198) | 1:90:A:GLU:H  | 1:90:A:GLU:HB2  | 34       | 0.15          |
| (3,144) | 1:101:A:LEU:H | 1:100:A:GLU:HB2 | 14       | 0.15          |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 6        | 0.15          |
| (3,113) | 1:63:A:CYS:H  | 1:60:A:ASP:H    | 16       | 0.15          |
| (3,102) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 3        | 0.15          |
| (3,72)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 15       | 0.15          |
| (3,59)  | 1:42:A:TRP:H  | 1:41:A:THR:HB   | 4        | 0.15          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,59)   | 1:42:A:TRP:H   | 1:41:A:THR:HB   | 6        | 0.15          |
| (3,59)   | 1:42:A:TRP:H   | 1:41:A:THR:HB   | 22       | 0.15          |
| (3,59)   | 1:42:A:TRP:H   | 1:41:A:THR:HB   | 33       | 0.15          |
| (3,51)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2  | 20       | 0.15          |
| (3,51)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2  | 34       | 0.15          |
| (3,51)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2  | 36       | 0.15          |
| (3,50)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 1        | 0.15          |
| (3,50)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 9        | 0.15          |
| (3,50)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 13       | 0.15          |
| (3,50)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 15       | 0.15          |
| (3,50)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 18       | 0.15          |
| (3,50)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 22       | 0.15          |
| (3,50)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 23       | 0.15          |
| (3,50)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 30       | 0.15          |
| (3,50)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 38       | 0.15          |
| (3,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 6        | 0.15          |
| (3,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 11       | 0.15          |
| (3,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 15       | 0.15          |
| (3,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 18       | 0.15          |
| (3,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 19       | 0.15          |
| (1,3211) | 1:69:A:HIS:HE1 | 1:67:A:THR:HB   | 15       | 0.15          |
| (1,3211) | 1:69:A:HIS:HE1 | 1:67:A:THR:HB   | 22       | 0.15          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 17       | 0.15          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 17       | 0.15          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 18       | 0.15          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 18       | 0.15          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 5        | 0.15          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 5        | 0.15          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 5        | 0.15          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 5        | 0.15          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 5        | 0.15          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 5        | 0.15          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 7        | 0.15          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 7        | 0.15          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 7        | 0.15          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 7        | 0.15          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 7        | 0.15          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 7        | 0.15          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 11       | 0.15          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 11       | 0.15          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 11       | 0.15          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 11       | 0.15          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 11       | 0.15          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 11       | 0.15          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 14       | 0.15          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 14       | 0.15          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 14       | 0.15          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 14       | 0.15          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 14       | 0.15          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 14       | 0.15          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 15       | 0.15          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 15       | 0.15          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 15       | 0.15          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 15       | 0.15          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 15       | 0.15          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 15       | 0.15          |
| (1,3199) | 1:43:A:TYR:HD1 | 1:80:A:SER:HB2  | 29       | 0.15          |
| (1,3199) | 1:43:A:TYR:HD2 | 1:80:A:SER:HB2  | 29       | 0.15          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 16       | 0.15          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 16       | 0.15          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 16       | 0.15          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 16       | 0.15          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 21       | 0.15          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 21       | 0.15          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 21       | 0.15          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 21       | 0.15          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 28       | 0.15          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 28       | 0.15          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 28       | 0.15          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 28       | 0.15          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 39       | 0.15          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 39       | 0.15          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 39       | 0.15          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 39       | 0.15          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 40       | 0.15          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 40       | 0.15          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 40       | 0.15          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 40       | 0.15          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 37       | 0.15          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 40       | 0.15          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 15       | 0.15          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 15       | 0.15          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 15       | 0.15          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 19       | 0.15          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2 | 19       | 0.15          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3 | 19       | 0.15          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1 | 21       | 0.15          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2 | 21       | 0.15          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3 | 21       | 0.15          |
| (1,3137) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3 | 1        | 0.15          |
| (1,3137) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3 | 1        | 0.15          |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 11       | 0.15          |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 11       | 0.15          |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 16       | 0.15          |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 16       | 0.15          |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 26       | 0.15          |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 26       | 0.15          |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 27       | 0.15          |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 27       | 0.15          |
| (1,3132) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB2 | 10       | 0.15          |
| (1,3132) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB2 | 10       | 0.15          |
| (1,3131) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3 | 1        | 0.15          |
| (1,3131) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3 | 1        | 0.15          |
| (1,3131) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3 | 7        | 0.15          |
| (1,3131) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3 | 7        | 0.15          |
| (1,3131) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3 | 36       | 0.15          |
| (1,3131) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3 | 36       | 0.15          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 4        | 0.15          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 4        | 0.15          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 12       | 0.15          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 12       | 0.15          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 13       | 0.15          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 13       | 0.15          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 14       | 0.15          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 14       | 0.15          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 15       | 0.15          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 15       | 0.15          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 17       | 0.15          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 17       | 0.15          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 19       | 0.15          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 19       | 0.15          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 25       | 0.15          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 25       | 0.15          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 30       | 0.15          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA  | 30       | 0.15          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA  | 36       | 0.15          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 36       | 0.15          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 37       | 0.15          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 37       | 0.15          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 4        | 0.15          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 4        | 0.15          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 12       | 0.15          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 12       | 0.15          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 13       | 0.15          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 13       | 0.15          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 14       | 0.15          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 14       | 0.15          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 15       | 0.15          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 15       | 0.15          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 17       | 0.15          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 17       | 0.15          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 19       | 0.15          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 19       | 0.15          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 25       | 0.15          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 25       | 0.15          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 30       | 0.15          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 30       | 0.15          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 36       | 0.15          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 36       | 0.15          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 37       | 0.15          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 37       | 0.15          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 2        | 0.15          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 2        | 0.15          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 2        | 0.15          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 2        | 0.15          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 2        | 0.15          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 2        | 0.15          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 4        | 0.15          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 4        | 0.15          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 4        | 0.15          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 4        | 0.15          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 4        | 0.15          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 4        | 0.15          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 31       | 0.15          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 31       | 0.15          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 31       | 0.15          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 31       | 0.15          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 31       | 0.15          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 31       | 0.15          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 32       | 0.15          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 32       | 0.15          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 32       | 0.15          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 32       | 0.15          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 32       | 0.15          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 32       | 0.15          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 34       | 0.15          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 34       | 0.15          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 34       | 0.15          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 34       | 0.15          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 34       | 0.15          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 34       | 0.15          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 36       | 0.15          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 36       | 0.15          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 36       | 0.15          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 36       | 0.15          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 36       | 0.15          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 36       | 0.15          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 37       | 0.15          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 37       | 0.15          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 37       | 0.15          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 37       | 0.15          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 37       | 0.15          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 37       | 0.15          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 11       | 0.15          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 11       | 0.15          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 11       | 0.15          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 11       | 0.15          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 11       | 0.15          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 11       | 0.15          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 17       | 0.15          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 17       | 0.15          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 17       | 0.15          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 17       | 0.15          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 17       | 0.15          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 17       | 0.15          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 25       | 0.15          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 25       | 0.15          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 25       | 0.15          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 25       | 0.15          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 25       | 0.15          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 25       | 0.15          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 27       | 0.15          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 27       | 0.15          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 27       | 0.15          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 27       | 0.15          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 27       | 0.15          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 27       | 0.15          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 30       | 0.15          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 30       | 0.15          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 30       | 0.15          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 30       | 0.15          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 30       | 0.15          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 30       | 0.15          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 8        | 0.15          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 8        | 0.15          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 8        | 0.15          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 8        | 0.15          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 22       | 0.15          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 22       | 0.15          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 22       | 0.15          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 22       | 0.15          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 37       | 0.15          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 37       | 0.15          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 37       | 0.15          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 37       | 0.15          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 7        | 0.15          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 7        | 0.15          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 7        | 0.15          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 7        | 0.15          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 7        | 0.15          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 7        | 0.15          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 9        | 0.15          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 9        | 0.15          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 9        | 0.15          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 9        | 0.15          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 9        | 0.15          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 9        | 0.15          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 10       | 0.15          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 10       | 0.15          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 10       | 0.15          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 10       | 0.15          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 10       | 0.15          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 10       | 0.15          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 16       | 0.15          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 16       | 0.15          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 16       | 0.15          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 16       | 0.15          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 16       | 0.15          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 16       | 0.15          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 24       | 0.15          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 24       | 0.15          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 24       | 0.15          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 24       | 0.15          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 24       | 0.15          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 24       | 0.15          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 39       | 0.15          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 39       | 0.15          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 39       | 0.15          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 39       | 0.15          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 39       | 0.15          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 39       | 0.15          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 10       | 0.15          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 10       | 0.15          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 10       | 0.15          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 24       | 0.15          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 24       | 0.15          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 24       | 0.15          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 31       | 0.15          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 31       | 0.15          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 31       | 0.15          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 1        | 0.15          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 1        | 0.15          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 3        | 0.15          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 3        | 0.15          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 17       | 0.15          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 17       | 0.15          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 22       | 0.15          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 22       | 0.15          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 26       | 0.15          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 26       | 0.15          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 31       | 0.15          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 31       | 0.15          |
| (1,3040) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG21 | 10       | 0.15          |
| (1,3040) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG22 | 10       | 0.15          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3040) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG23 | 10       | 0.15          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 22       | 0.15          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 22       | 0.15          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 22       | 0.15          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 23       | 0.15          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 23       | 0.15          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 23       | 0.15          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 31       | 0.15          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 31       | 0.15          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 31       | 0.15          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 19       | 0.15          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 19       | 0.15          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 19       | 0.15          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 26       | 0.15          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 26       | 0.15          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 26       | 0.15          |
| (1,2996) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 10       | 0.15          |
| (1,2996) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 15       | 0.15          |
| (1,2996) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 27       | 0.15          |
| (1,2974) | 1:65:A:TYR:HA  | 1:42:A:TRP:HZ2  | 15       | 0.15          |
| (1,2974) | 1:65:A:TYR:HA  | 1:42:A:TRP:HZ2  | 16       | 0.15          |
| (1,2962) | 1:44:A:LYS:HE2 | 1:44:A:LYS:HG3  | 35       | 0.15          |
| (1,2949) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA    | 3        | 0.15          |
| (1,2949) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA    | 25       | 0.15          |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1  | 1        | 0.15          |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2  | 1        | 0.15          |
| (1,2931) | 1:26:A:SER:HA  | 1:70:A:ASN:H    | 3        | 0.15          |
| (1,2931) | 1:26:A:SER:HA  | 1:70:A:ASN:H    | 25       | 0.15          |
| (1,2929) | 1:17:A:GLN:HG2 | 1:17:A:GLN:H    | 5        | 0.15          |
| (1,2929) | 1:17:A:GLN:HG2 | 1:17:A:GLN:H    | 26       | 0.15          |
| (1,2918) | 1:22:A:SER:HB2 | 1:25:A:GLN:H    | 34       | 0.15          |
| (1,2903) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD2  | 2        | 0.15          |
| (1,2903) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD2  | 3        | 0.15          |
| (1,2903) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD2  | 5        | 0.15          |
| (1,2903) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD2  | 14       | 0.15          |
| (1,2903) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD2  | 15       | 0.15          |
| (1,2903) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD2  | 22       | 0.15          |
| (1,2859) | 1:92:A:ARG:HB3 | 1:92:A:ARG:H    | 2        | 0.15          |
| (1,2859) | 1:92:A:ARG:HB3 | 1:92:A:ARG:H    | 4        | 0.15          |
| (1,2859) | 1:92:A:ARG:HB3 | 1:92:A:ARG:H    | 6        | 0.15          |
| (1,2859) | 1:92:A:ARG:HB3 | 1:92:A:ARG:H    | 11       | 0.15          |
| (1,2859) | 1:92:A:ARG:HB3 | 1:92:A:ARG:H    | 13       | 0.15          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (1,2859) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H  | 19       | 0.15          |
| (1,2859) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H  | 22       | 0.15          |
| (1,2859) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H  | 23       | 0.15          |
| (1,2859) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H  | 31       | 0.15          |
| (1,2859) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H  | 37       | 0.15          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H | 9        | 0.15          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H | 16       | 0.15          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H | 24       | 0.15          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H | 34       | 0.15          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H | 39       | 0.15          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H | 40       | 0.15          |
| (1,2754) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H  | 3        | 0.15          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 1        | 0.15          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 2        | 0.15          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 10       | 0.15          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 11       | 0.15          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 18       | 0.15          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 21       | 0.15          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 24       | 0.15          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 31       | 0.15          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 32       | 0.15          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 33       | 0.15          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 34       | 0.15          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H  | 40       | 0.15          |
| (1,2686) | 1:8:A:GLU:HB3   | 1:8:A:GLU:HG2 | 1        | 0.15          |
| (1,2686) | 1:8:A:GLU:HB3   | 1:8:A:GLU:HG2 | 11       | 0.15          |
| (1,2686) | 1:8:A:GLU:HB3   | 1:8:A:GLU:HG2 | 23       | 0.15          |
| (1,2686) | 1:8:A:GLU:HB3   | 1:8:A:GLU:HG2 | 32       | 0.15          |
| (1,2675) | 1:25:A:GLN:HG3  | 1:26:A:SER:H  | 3        | 0.15          |
| (1,2675) | 1:25:A:GLN:HG3  | 1:26:A:SER:H  | 16       | 0.15          |
| (1,2675) | 1:25:A:GLN:HG3  | 1:26:A:SER:H  | 21       | 0.15          |
| (1,2675) | 1:25:A:GLN:HG3  | 1:26:A:SER:H  | 25       | 0.15          |
| (1,2675) | 1:25:A:GLN:HG3  | 1:26:A:SER:H  | 29       | 0.15          |
| (1,2675) | 1:25:A:GLN:HG3  | 1:26:A:SER:H  | 33       | 0.15          |
| (1,2675) | 1:25:A:GLN:HG3  | 1:26:A:SER:H  | 34       | 0.15          |
| (1,2675) | 1:25:A:GLN:HG3  | 1:26:A:SER:H  | 35       | 0.15          |
| (1,2675) | 1:25:A:GLN:HG3  | 1:26:A:SER:H  | 36       | 0.15          |
| (1,2675) | 1:25:A:GLN:HG3  | 1:26:A:SER:H  | 38       | 0.15          |
| (1,2653) | 1:17:A:GLN:HG2  | 1:17:A:GLN:HA | 8        | 0.15          |
| (1,2646) | 1:9:A:PRO:HB2   | 1:9:A:PRO:HD3 | 28       | 0.15          |
| (1,2645) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3 | 26       | 0.15          |
| (1,2645) | 1:9:A:PRO:HB3   | 1:9:A:PRO:HD3 | 27       | 0.15          |

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| Key      | Atom-1         | Atom-2        | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3 | 29       | 0.15          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3 | 37       | 0.15          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3 | 40       | 0.15          |
| (1,2550) | 1:92:A:ARG:HA  | 1:83:A:ALA:H  | 23       | 0.15          |
| (1,2550) | 1:92:A:ARG:HA  | 1:83:A:ALA:H  | 27       | 0.15          |
| (1,2550) | 1:92:A:ARG:HA  | 1:83:A:ALA:H  | 40       | 0.15          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA | 1        | 0.15          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA | 3        | 0.15          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA | 5        | 0.15          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA | 9        | 0.15          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA | 10       | 0.15          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA | 13       | 0.15          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA | 14       | 0.15          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA | 19       | 0.15          |
| (1,2537) | 1:73:A:PRO:HG3 | 1:73:A:PRO:HA | 23       | 0.15          |
| (1,2537) | 1:73:A:PRO:HG3 | 1:73:A:PRO:HA | 37       | 0.15          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 1        | 0.15          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 2        | 0.15          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 3        | 0.15          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 4        | 0.15          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 5        | 0.15          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 6        | 0.15          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 7        | 0.15          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 9        | 0.15          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 10       | 0.15          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 11       | 0.15          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 12       | 0.15          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 13       | 0.15          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 14       | 0.15          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 15       | 0.15          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 16       | 0.15          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 18       | 0.15          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 19       | 0.15          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 20       | 0.15          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 1        | 0.15          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 2        | 0.15          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 4        | 0.15          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 8        | 0.15          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 9        | 0.15          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 10       | 0.15          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 13       | 0.15          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 15       | 0.15          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,2491) | 1:9:A:PRO:HB2 | 1:9:A:PRO:HA  | 16       | 0.15          |
| (1,2491) | 1:9:A:PRO:HB2 | 1:9:A:PRO:HA  | 17       | 0.15          |
| (1,2491) | 1:9:A:PRO:HB2 | 1:9:A:PRO:HA  | 18       | 0.15          |
| (1,2491) | 1:9:A:PRO:HB2 | 1:9:A:PRO:HA  | 19       | 0.15          |
| (1,2491) | 1:9:A:PRO:HB2 | 1:9:A:PRO:HA  | 20       | 0.15          |
| (1,2485) | 1:9:A:PRO:HD2 | 1:9:A:PRO:HB3 | 2        | 0.15          |
| (1,2485) | 1:9:A:PRO:HD2 | 1:9:A:PRO:HB3 | 7        | 0.15          |
| (1,2485) | 1:9:A:PRO:HD2 | 1:9:A:PRO:HB3 | 9        | 0.15          |
| (1,2485) | 1:9:A:PRO:HD2 | 1:9:A:PRO:HB3 | 10       | 0.15          |
| (1,2485) | 1:9:A:PRO:HD2 | 1:9:A:PRO:HB3 | 11       | 0.15          |
| (1,2485) | 1:9:A:PRO:HD2 | 1:9:A:PRO:HB3 | 12       | 0.15          |
| (1,2485) | 1:9:A:PRO:HD2 | 1:9:A:PRO:HB3 | 13       | 0.15          |
| (1,2485) | 1:9:A:PRO:HD2 | 1:9:A:PRO:HB3 | 15       | 0.15          |
| (1,2485) | 1:9:A:PRO:HD2 | 1:9:A:PRO:HB3 | 18       | 0.15          |
| (1,2485) | 1:9:A:PRO:HD2 | 1:9:A:PRO:HB3 | 20       | 0.15          |
| (1,2479) | 1:9:A:PRO:HD2 | 1:8:A:GLU:HA  | 2        | 0.15          |
| (1,2479) | 1:9:A:PRO:HD2 | 1:8:A:GLU:HA  | 10       | 0.15          |
| (1,2479) | 1:9:A:PRO:HD2 | 1:8:A:GLU:HA  | 18       | 0.15          |
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 2        | 0.15          |
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 3        | 0.15          |
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 5        | 0.15          |
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 6        | 0.15          |
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 7        | 0.15          |
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 8        | 0.15          |
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 11       | 0.15          |
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 13       | 0.15          |
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 14       | 0.15          |
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 19       | 0.15          |
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 20       | 0.15          |
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 21       | 0.15          |
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 22       | 0.15          |
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 23       | 0.15          |
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 24       | 0.15          |
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 25       | 0.15          |
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 26       | 0.15          |
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 27       | 0.15          |
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 28       | 0.15          |
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 29       | 0.15          |
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 30       | 0.15          |
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 31       | 0.15          |
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 32       | 0.15          |
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 33       | 0.15          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 34       | 0.15          |
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 36       | 0.15          |
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 37       | 0.15          |
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 38       | 0.15          |
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 39       | 0.15          |
| (1,2475) | 1:4:A:PRO:HG3 | 1:4:A:PRO:HG2 | 40       | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 2        | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 3        | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 5        | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 6        | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 7        | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 8        | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 11       | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 13       | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 14       | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 19       | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 20       | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 21       | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 22       | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 23       | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 24       | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 25       | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 26       | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 27       | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 28       | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 29       | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 30       | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 31       | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 32       | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 33       | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 34       | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 36       | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 37       | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 38       | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 39       | 0.15          |
| (1,2474) | 1:4:A:PRO:HG2 | 1:4:A:PRO:HG3 | 40       | 0.15          |
| (1,2460) | 1:4:A:PRO:HD3 | 1:3:A:ASP:HA  | 14       | 0.15          |
| (1,2460) | 1:4:A:PRO:HD3 | 1:3:A:ASP:HA  | 23       | 0.15          |
| (1,2431) | 1:82:A:ILE:HB | 1:41:A:THR:H  | 4        | 0.15          |
| (1,2431) | 1:82:A:ILE:HB | 1:41:A:THR:H  | 21       | 0.15          |
| (1,2431) | 1:82:A:ILE:HB | 1:41:A:THR:H  | 22       | 0.15          |
| (1,2431) | 1:82:A:ILE:HB | 1:41:A:THR:H  | 24       | 0.15          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,2431) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 25       | 0.15          |
| (1,2416) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA   | 32       | 0.15          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 4        | 0.15          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 6        | 0.15          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 11       | 0.15          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 12       | 0.15          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 14       | 0.15          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 16       | 0.15          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 20       | 0.15          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 21       | 0.15          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 23       | 0.15          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 25       | 0.15          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 32       | 0.15          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 37       | 0.15          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 39       | 0.15          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 40       | 0.15          |
| (1,2403) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 1        | 0.15          |
| (1,2403) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 1        | 0.15          |
| (1,2403) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 1        | 0.15          |
| (1,2403) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 3        | 0.15          |
| (1,2403) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 3        | 0.15          |
| (1,2403) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 3        | 0.15          |
| (1,2403) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 8        | 0.15          |
| (1,2403) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 8        | 0.15          |
| (1,2403) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 8        | 0.15          |
| (1,2403) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 11       | 0.15          |
| (1,2403) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 11       | 0.15          |
| (1,2403) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 11       | 0.15          |
| (1,2403) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 17       | 0.15          |
| (1,2403) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 17       | 0.15          |
| (1,2403) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 17       | 0.15          |
| (1,2403) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 20       | 0.15          |
| (1,2403) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 20       | 0.15          |
| (1,2403) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 20       | 0.15          |
| (1,2403) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 22       | 0.15          |
| (1,2403) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 22       | 0.15          |
| (1,2403) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 22       | 0.15          |
| (1,2403) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 23       | 0.15          |
| (1,2403) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 23       | 0.15          |
| (1,2403) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 23       | 0.15          |
| (1,2403) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 25       | 0.15          |
| (1,2403) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 25       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2403) | 1:66:A:MET:HE3  | 1:42:A:TRP:H    | 25       | 0.15          |
| (1,2403) | 1:66:A:MET:HE1  | 1:42:A:TRP:H    | 26       | 0.15          |
| (1,2403) | 1:66:A:MET:HE2  | 1:42:A:TRP:H    | 26       | 0.15          |
| (1,2403) | 1:66:A:MET:HE3  | 1:42:A:TRP:H    | 26       | 0.15          |
| (1,2403) | 1:66:A:MET:HE1  | 1:42:A:TRP:H    | 30       | 0.15          |
| (1,2403) | 1:66:A:MET:HE2  | 1:42:A:TRP:H    | 30       | 0.15          |
| (1,2403) | 1:66:A:MET:HE3  | 1:42:A:TRP:H    | 30       | 0.15          |
| (1,2402) | 1:66:A:MET:HE1  | 1:29:A:PHE:HZ   | 9        | 0.15          |
| (1,2402) | 1:66:A:MET:HE2  | 1:29:A:PHE:HZ   | 9        | 0.15          |
| (1,2402) | 1:66:A:MET:HE3  | 1:29:A:PHE:HZ   | 9        | 0.15          |
| (1,2402) | 1:66:A:MET:HE1  | 1:29:A:PHE:HZ   | 13       | 0.15          |
| (1,2402) | 1:66:A:MET:HE2  | 1:29:A:PHE:HZ   | 13       | 0.15          |
| (1,2402) | 1:66:A:MET:HE3  | 1:29:A:PHE:HZ   | 13       | 0.15          |
| (1,2402) | 1:66:A:MET:HE1  | 1:29:A:PHE:HZ   | 37       | 0.15          |
| (1,2402) | 1:66:A:MET:HE2  | 1:29:A:PHE:HZ   | 37       | 0.15          |
| (1,2402) | 1:66:A:MET:HE3  | 1:29:A:PHE:HZ   | 37       | 0.15          |
| (1,2287) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 7        | 0.15          |
| (1,2287) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 12       | 0.15          |
| (1,2287) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 17       | 0.15          |
| (1,2287) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 18       | 0.15          |
| (1,2287) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 22       | 0.15          |
| (1,2287) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 34       | 0.15          |
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG21 | 8        | 0.15          |
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG22 | 8        | 0.15          |
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG23 | 8        | 0.15          |
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG21 | 20       | 0.15          |
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG22 | 20       | 0.15          |
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG23 | 20       | 0.15          |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD11 | 21       | 0.15          |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD12 | 21       | 0.15          |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD13 | 21       | 0.15          |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD11 | 25       | 0.15          |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD12 | 25       | 0.15          |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD13 | 25       | 0.15          |
| (1,2145) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 24       | 0.15          |
| (1,2105) | 1:16:A:ILE:HD11 | 1:95:A:ALA:HA   | 28       | 0.15          |
| (1,2105) | 1:16:A:ILE:HD12 | 1:95:A:ALA:HA   | 28       | 0.15          |
| (1,2105) | 1:16:A:ILE:HD13 | 1:95:A:ALA:HA   | 28       | 0.15          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 4        | 0.15          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 4        | 0.15          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 4        | 0.15          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 21       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 21       | 0.15          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 21       | 0.15          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 22       | 0.15          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 22       | 0.15          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 22       | 0.15          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 25       | 0.15          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 25       | 0.15          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 25       | 0.15          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 30       | 0.15          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 30       | 0.15          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 30       | 0.15          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 38       | 0.15          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 38       | 0.15          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 38       | 0.15          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1  | 3        | 0.15          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2  | 3        | 0.15          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1  | 3        | 0.15          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2  | 3        | 0.15          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1  | 3        | 0.15          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2  | 3        | 0.15          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1  | 9        | 0.15          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2  | 9        | 0.15          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1  | 9        | 0.15          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2  | 9        | 0.15          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1  | 9        | 0.15          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2  | 9        | 0.15          |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD11 | 2        | 0.15          |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD12 | 2        | 0.15          |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD13 | 2        | 0.15          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD11 | 2        | 0.15          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD12 | 2        | 0.15          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD13 | 2        | 0.15          |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD11 | 2        | 0.15          |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD12 | 2        | 0.15          |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD13 | 2        | 0.15          |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD11 | 11       | 0.15          |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD12 | 11       | 0.15          |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD13 | 11       | 0.15          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD11 | 11       | 0.15          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD12 | 11       | 0.15          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD13 | 11       | 0.15          |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD11 | 11       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD12 | 11       | 0.15          |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD13 | 11       | 0.15          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3  | 3        | 0.15          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3  | 3        | 0.15          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3  | 3        | 0.15          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3  | 8        | 0.15          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3  | 8        | 0.15          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3  | 8        | 0.15          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3  | 9        | 0.15          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3  | 9        | 0.15          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3  | 9        | 0.15          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 5        | 0.15          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 5        | 0.15          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 5        | 0.15          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 13       | 0.15          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 13       | 0.15          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 13       | 0.15          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 30       | 0.15          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 30       | 0.15          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 30       | 0.15          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 36       | 0.15          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 36       | 0.15          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 36       | 0.15          |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3  | 15       | 0.15          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3  | 15       | 0.15          |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3  | 15       | 0.15          |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3  | 38       | 0.15          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3  | 38       | 0.15          |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3  | 38       | 0.15          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1  | 18       | 0.15          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2  | 18       | 0.15          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1  | 18       | 0.15          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2  | 18       | 0.15          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1  | 18       | 0.15          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2  | 18       | 0.15          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1  | 32       | 0.15          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2  | 32       | 0.15          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1  | 32       | 0.15          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2  | 32       | 0.15          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1  | 32       | 0.15          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2  | 32       | 0.15          |
| (1,2014) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD1  | 18       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2014) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD2  | 18       | 0.15          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1  | 4        | 0.15          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2  | 4        | 0.15          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3  | 4        | 0.15          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1  | 4        | 0.15          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2  | 4        | 0.15          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3  | 4        | 0.15          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1  | 4        | 0.15          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2  | 4        | 0.15          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3  | 4        | 0.15          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 9        | 0.15          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 15       | 0.15          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 20       | 0.15          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 23       | 0.15          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 26       | 0.15          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 32       | 0.15          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 34       | 0.15          |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 22       | 0.15          |
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 22       | 0.15          |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 22       | 0.15          |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 25       | 0.15          |
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 25       | 0.15          |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 25       | 0.15          |
| (1,1990) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 8        | 0.15          |
| (1,1990) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 8        | 0.15          |
| (1,1990) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 8        | 0.15          |
| (1,1990) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 12       | 0.15          |
| (1,1990) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 12       | 0.15          |
| (1,1990) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 12       | 0.15          |
| (1,1990) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 18       | 0.15          |
| (1,1990) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 18       | 0.15          |
| (1,1990) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 18       | 0.15          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 2        | 0.15          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 7        | 0.15          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 8        | 0.15          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 13       | 0.15          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 22       | 0.15          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 26       | 0.15          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 31       | 0.15          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 32       | 0.15          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 33       | 0.15          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 35       | 0.15          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA | 38       | 0.15          |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA | 6        | 0.15          |
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA | 6        | 0.15          |
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA | 6        | 0.15          |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA | 8        | 0.15          |
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA | 8        | 0.15          |
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA | 8        | 0.15          |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA | 17       | 0.15          |
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA | 17       | 0.15          |
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA | 17       | 0.15          |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA | 20       | 0.15          |
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA | 20       | 0.15          |
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA | 20       | 0.15          |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA | 22       | 0.15          |
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA | 22       | 0.15          |
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA | 22       | 0.15          |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA | 30       | 0.15          |
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA | 30       | 0.15          |
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA | 30       | 0.15          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 5        | 0.15          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 5        | 0.15          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 5        | 0.15          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 8        | 0.15          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 8        | 0.15          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 8        | 0.15          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 10       | 0.15          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 10       | 0.15          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 10       | 0.15          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 12       | 0.15          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 12       | 0.15          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 12       | 0.15          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 13       | 0.15          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 13       | 0.15          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 13       | 0.15          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 14       | 0.15          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 14       | 0.15          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 14       | 0.15          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 15       | 0.15          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 15       | 0.15          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 15       | 0.15          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 18       | 0.15          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 18       | 0.15          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 18       | 0.15          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 21       | 0.15          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 21       | 0.15          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 21       | 0.15          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 22       | 0.15          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 22       | 0.15          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 22       | 0.15          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 23       | 0.15          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 23       | 0.15          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 23       | 0.15          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 26       | 0.15          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 26       | 0.15          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 26       | 0.15          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 30       | 0.15          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 30       | 0.15          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 30       | 0.15          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 31       | 0.15          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 31       | 0.15          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 31       | 0.15          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 32       | 0.15          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 32       | 0.15          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 32       | 0.15          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 33       | 0.15          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 33       | 0.15          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 33       | 0.15          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 34       | 0.15          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 34       | 0.15          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 34       | 0.15          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 37       | 0.15          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 37       | 0.15          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 37       | 0.15          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 39       | 0.15          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 39       | 0.15          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 39       | 0.15          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H  | 40       | 0.15          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H  | 40       | 0.15          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H  | 40       | 0.15          |
| (1,1863) | 1:7:A:ALA:HB1   | 1:8:A:GLU:H   | 16       | 0.15          |
| (1,1863) | 1:7:A:ALA:HB2   | 1:8:A:GLU:H   | 16       | 0.15          |
| (1,1863) | 1:7:A:ALA:HB3   | 1:8:A:GLU:H   | 16       | 0.15          |
| (1,1861) | 1:7:A:ALA:HB1   | 1:88:A:ARG:HA | 26       | 0.15          |
| (1,1861) | 1:7:A:ALA:HB2   | 1:88:A:ARG:HA | 26       | 0.15          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1861) | 1:7:A:ALA:HB3  | 1:88:A:ARG:HA  | 26       | 0.15          |
| (1,1853) | 1:27:A:ALA:HB1 | 1:28:A:THR:H   | 4        | 0.15          |
| (1,1853) | 1:27:A:ALA:HB2 | 1:28:A:THR:H   | 4        | 0.15          |
| (1,1853) | 1:27:A:ALA:HB3 | 1:28:A:THR:H   | 4        | 0.15          |
| (1,1853) | 1:27:A:ALA:HB1 | 1:28:A:THR:H   | 10       | 0.15          |
| (1,1853) | 1:27:A:ALA:HB2 | 1:28:A:THR:H   | 10       | 0.15          |
| (1,1853) | 1:27:A:ALA:HB3 | 1:28:A:THR:H   | 10       | 0.15          |
| (1,1853) | 1:27:A:ALA:HB1 | 1:28:A:THR:H   | 14       | 0.15          |
| (1,1853) | 1:27:A:ALA:HB2 | 1:28:A:THR:H   | 14       | 0.15          |
| (1,1853) | 1:27:A:ALA:HB3 | 1:28:A:THR:H   | 14       | 0.15          |
| (1,1853) | 1:27:A:ALA:HB1 | 1:28:A:THR:H   | 18       | 0.15          |
| (1,1853) | 1:27:A:ALA:HB2 | 1:28:A:THR:H   | 18       | 0.15          |
| (1,1853) | 1:27:A:ALA:HB3 | 1:28:A:THR:H   | 18       | 0.15          |
| (1,1853) | 1:27:A:ALA:HB1 | 1:28:A:THR:H   | 28       | 0.15          |
| (1,1853) | 1:27:A:ALA:HB2 | 1:28:A:THR:H   | 28       | 0.15          |
| (1,1853) | 1:27:A:ALA:HB3 | 1:28:A:THR:H   | 28       | 0.15          |
| (1,1853) | 1:27:A:ALA:HB1 | 1:28:A:THR:H   | 34       | 0.15          |
| (1,1853) | 1:27:A:ALA:HB2 | 1:28:A:THR:H   | 34       | 0.15          |
| (1,1853) | 1:27:A:ALA:HB3 | 1:28:A:THR:H   | 34       | 0.15          |
| (1,1853) | 1:27:A:ALA:HB1 | 1:28:A:THR:H   | 39       | 0.15          |
| (1,1853) | 1:27:A:ALA:HB2 | 1:28:A:THR:H   | 39       | 0.15          |
| (1,1853) | 1:27:A:ALA:HB3 | 1:28:A:THR:H   | 39       | 0.15          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2 | 1        | 0.15          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2 | 9        | 0.15          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2 | 12       | 0.15          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3 | 2        | 0.15          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3 | 3        | 0.15          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3 | 11       | 0.15          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3 | 12       | 0.15          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3 | 14       | 0.15          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3 | 16       | 0.15          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3 | 17       | 0.15          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3 | 20       | 0.15          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3 | 24       | 0.15          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3 | 26       | 0.15          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3 | 28       | 0.15          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3 | 33       | 0.15          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3 | 34       | 0.15          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3 | 35       | 0.15          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3 | 37       | 0.15          |
| (1,1778) | 1:88:A:ARG:HG2 | 1:88:A:ARG:H   | 26       | 0.15          |
| (1,1744) | 1:51:A:GLU:HG2 | 1:51:A:GLU:H   | 15       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG11 | 10       | 0.15          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG12 | 10       | 0.15          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG13 | 10       | 0.15          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG11 | 10       | 0.15          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG12 | 10       | 0.15          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 10       | 0.15          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 10       | 0.15          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 10       | 0.15          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 10       | 0.15          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG11 | 27       | 0.15          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG12 | 27       | 0.15          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG13 | 27       | 0.15          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG11 | 27       | 0.15          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG12 | 27       | 0.15          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 27       | 0.15          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 27       | 0.15          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 27       | 0.15          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 27       | 0.15          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG11 | 28       | 0.15          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG12 | 28       | 0.15          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG13 | 28       | 0.15          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG11 | 28       | 0.15          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG12 | 28       | 0.15          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 28       | 0.15          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 28       | 0.15          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 28       | 0.15          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 28       | 0.15          |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 13       | 0.15          |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 13       | 0.15          |
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 13       | 0.15          |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 31       | 0.15          |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 31       | 0.15          |
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 31       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 15       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 15       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 15       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 15       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 15       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 15       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 15       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 15       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 15       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 17       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 17       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 17       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 17       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 17       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 17       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 17       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 17       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 17       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 24       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 24       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 24       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 24       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 24       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 24       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 24       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 24       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 24       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 32       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 32       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 32       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 32       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 32       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 32       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 32       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 32       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 32       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 37       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 37       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 37       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 37       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 37       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 37       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 37       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 37       | 0.15          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 37       | 0.15          |
| (1,1679) | 1:85:A:LEU:HD11 | 1:35:A:PHE:HD1  | 1        | 0.15          |
| (1,1679) | 1:85:A:LEU:HD11 | 1:35:A:PHE:HD2  | 1        | 0.15          |
| (1,1679) | 1:85:A:LEU:HD12 | 1:35:A:PHE:HD1  | 1        | 0.15          |
| (1,1679) | 1:85:A:LEU:HD12 | 1:35:A:PHE:HD2  | 1        | 0.15          |
| (1,1679) | 1:85:A:LEU:HD13 | 1:35:A:PHE:HD1  | 1        | 0.15          |
| (1,1679) | 1:85:A:LEU:HD13 | 1:35:A:PHE:HD2  | 1        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 22       | 0.15          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 22       | 0.15          |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 22       | 0.15          |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 28       | 0.15          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 28       | 0.15          |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 28       | 0.15          |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 31       | 0.15          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 31       | 0.15          |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 31       | 0.15          |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 36       | 0.15          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 36       | 0.15          |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 36       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 18       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 18       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 18       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 18       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 18       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 18       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 18       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 18       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 18       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 21       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 21       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 21       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 21       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 21       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 21       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 21       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 21       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 21       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 31       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 31       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 31       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 31       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 31       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 31       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 31       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 31       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 31       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 33       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 33       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 33       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 33       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 33       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 33       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 33       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 33       | 0.15          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 33       | 0.15          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 14       | 0.15          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 14       | 0.15          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 14       | 0.15          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 15       | 0.15          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 15       | 0.15          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 15       | 0.15          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 19       | 0.15          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 19       | 0.15          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 19       | 0.15          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 25       | 0.15          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 25       | 0.15          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 25       | 0.15          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 29       | 0.15          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 29       | 0.15          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 29       | 0.15          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 39       | 0.15          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 39       | 0.15          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 39       | 0.15          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 40       | 0.15          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 40       | 0.15          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 40       | 0.15          |
| (1,1624) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2  | 29       | 0.15          |
| (1,1624) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2  | 29       | 0.15          |
| (1,1624) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2  | 29       | 0.15          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 11       | 0.15          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 11       | 0.15          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 11       | 0.15          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 15       | 0.15          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 15       | 0.15          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 15       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1  | 2        | 0.15          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2  | 2        | 0.15          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1  | 2        | 0.15          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2  | 2        | 0.15          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1  | 2        | 0.15          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2  | 2        | 0.15          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 4        | 0.15          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 4        | 0.15          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 4        | 0.15          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 4        | 0.15          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 4        | 0.15          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 4        | 0.15          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 31       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 31       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 31       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 31       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 31       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 31       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 32       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 32       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 32       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 32       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 32       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 32       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 34       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 34       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 34       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 34       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 34       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 34       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 36       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 36       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 36       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 36       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 36       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 36       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 37       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 37       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 37       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 37       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 37       | 0.15          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 37       | 0.15          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 7        | 0.15          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 7        | 0.15          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 7        | 0.15          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 7        | 0.15          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 7        | 0.15          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 7        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 11       | 0.15          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 11       | 0.15          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 11       | 0.15          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 11       | 0.15          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 11       | 0.15          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 11       | 0.15          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 26       | 0.15          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 26       | 0.15          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 26       | 0.15          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 26       | 0.15          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 26       | 0.15          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 26       | 0.15          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 28       | 0.15          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 28       | 0.15          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 28       | 0.15          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 28       | 0.15          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 28       | 0.15          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 28       | 0.15          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 4        | 0.15          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 4        | 0.15          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 4        | 0.15          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 12       | 0.15          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 12       | 0.15          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 12       | 0.15          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 14       | 0.15          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 14       | 0.15          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 14       | 0.15          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 21       | 0.15          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 21       | 0.15          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 21       | 0.15          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 30       | 0.15          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 30       | 0.15          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 30       | 0.15          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 40       | 0.15          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 40       | 0.15          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 40       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 6        | 0.15          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 6        | 0.15          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 6        | 0.15          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 10       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 10       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 10       | 0.15          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA | 11       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA | 11       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA | 11       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA | 13       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA | 13       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA | 13       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA | 14       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA | 14       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA | 14       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA | 15       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA | 15       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA | 15       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA | 22       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA | 22       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA | 22       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA | 26       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA | 26       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA | 26       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA | 30       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA | 30       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA | 30       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA | 34       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA | 34       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA | 34       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA | 37       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA | 37       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA | 37       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA | 40       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA | 40       | 0.15          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA | 40       | 0.15          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H  | 4        | 0.15          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H  | 4        | 0.15          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H  | 4        | 0.15          |
| (1,1514) | 1:66:A:MET:HE1  | 1:66:A:MET:H  | 3        | 0.15          |
| (1,1514) | 1:66:A:MET:HE2  | 1:66:A:MET:H  | 3        | 0.15          |
| (1,1514) | 1:66:A:MET:HE3  | 1:66:A:MET:H  | 3        | 0.15          |
| (1,1514) | 1:66:A:MET:HE1  | 1:66:A:MET:H  | 4        | 0.15          |
| (1,1514) | 1:66:A:MET:HE2  | 1:66:A:MET:H  | 4        | 0.15          |
| (1,1514) | 1:66:A:MET:HE3  | 1:66:A:MET:H  | 4        | 0.15          |
| (1,1514) | 1:66:A:MET:HE1  | 1:66:A:MET:H  | 5        | 0.15          |
| (1,1514) | 1:66:A:MET:HE2  | 1:66:A:MET:H  | 5        | 0.15          |
| (1,1514) | 1:66:A:MET:HE3  | 1:66:A:MET:H  | 5        | 0.15          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1514) | 1:66:A:MET:HE1 | 1:66:A:MET:H   | 8        | 0.15          |
| (1,1514) | 1:66:A:MET:HE2 | 1:66:A:MET:H   | 8        | 0.15          |
| (1,1514) | 1:66:A:MET:HE3 | 1:66:A:MET:H   | 8        | 0.15          |
| (1,1514) | 1:66:A:MET:HE1 | 1:66:A:MET:H   | 9        | 0.15          |
| (1,1514) | 1:66:A:MET:HE2 | 1:66:A:MET:H   | 9        | 0.15          |
| (1,1514) | 1:66:A:MET:HE3 | 1:66:A:MET:H   | 9        | 0.15          |
| (1,1514) | 1:66:A:MET:HE1 | 1:66:A:MET:H   | 15       | 0.15          |
| (1,1514) | 1:66:A:MET:HE2 | 1:66:A:MET:H   | 15       | 0.15          |
| (1,1514) | 1:66:A:MET:HE3 | 1:66:A:MET:H   | 15       | 0.15          |
| (1,1514) | 1:66:A:MET:HE1 | 1:66:A:MET:H   | 16       | 0.15          |
| (1,1514) | 1:66:A:MET:HE2 | 1:66:A:MET:H   | 16       | 0.15          |
| (1,1514) | 1:66:A:MET:HE3 | 1:66:A:MET:H   | 16       | 0.15          |
| (1,1514) | 1:66:A:MET:HE1 | 1:66:A:MET:H   | 17       | 0.15          |
| (1,1514) | 1:66:A:MET:HE2 | 1:66:A:MET:H   | 17       | 0.15          |
| (1,1514) | 1:66:A:MET:HE3 | 1:66:A:MET:H   | 17       | 0.15          |
| (1,1514) | 1:66:A:MET:HE1 | 1:66:A:MET:H   | 20       | 0.15          |
| (1,1514) | 1:66:A:MET:HE2 | 1:66:A:MET:H   | 20       | 0.15          |
| (1,1514) | 1:66:A:MET:HE3 | 1:66:A:MET:H   | 20       | 0.15          |
| (1,1514) | 1:66:A:MET:HE1 | 1:66:A:MET:H   | 32       | 0.15          |
| (1,1514) | 1:66:A:MET:HE2 | 1:66:A:MET:H   | 32       | 0.15          |
| (1,1514) | 1:66:A:MET:HE3 | 1:66:A:MET:H   | 32       | 0.15          |
| (1,1514) | 1:66:A:MET:HE1 | 1:66:A:MET:H   | 34       | 0.15          |
| (1,1514) | 1:66:A:MET:HE2 | 1:66:A:MET:H   | 34       | 0.15          |
| (1,1514) | 1:66:A:MET:HE3 | 1:66:A:MET:H   | 34       | 0.15          |
| (1,1514) | 1:66:A:MET:HE1 | 1:66:A:MET:H   | 35       | 0.15          |
| (1,1514) | 1:66:A:MET:HE2 | 1:66:A:MET:H   | 35       | 0.15          |
| (1,1514) | 1:66:A:MET:HE3 | 1:66:A:MET:H   | 35       | 0.15          |
| (1,1514) | 1:66:A:MET:HE1 | 1:66:A:MET:H   | 37       | 0.15          |
| (1,1514) | 1:66:A:MET:HE2 | 1:66:A:MET:H   | 37       | 0.15          |
| (1,1514) | 1:66:A:MET:HE3 | 1:66:A:MET:H   | 37       | 0.15          |
| (1,1513) | 1:66:A:MET:HE1 | 1:29:A:PHE:H   | 13       | 0.15          |
| (1,1513) | 1:66:A:MET:HE2 | 1:29:A:PHE:H   | 13       | 0.15          |
| (1,1513) | 1:66:A:MET:HE3 | 1:29:A:PHE:H   | 13       | 0.15          |
| (1,1513) | 1:66:A:MET:HE1 | 1:29:A:PHE:H   | 20       | 0.15          |
| (1,1513) | 1:66:A:MET:HE2 | 1:29:A:PHE:H   | 20       | 0.15          |
| (1,1513) | 1:66:A:MET:HE3 | 1:29:A:PHE:H   | 20       | 0.15          |
| (1,1510) | 1:66:A:MET:HE1 | 1:42:A:TRP:HE1 | 15       | 0.15          |
| (1,1510) | 1:66:A:MET:HE2 | 1:42:A:TRP:HE1 | 15       | 0.15          |
| (1,1510) | 1:66:A:MET:HE3 | 1:42:A:TRP:HE1 | 15       | 0.15          |
| (1,1510) | 1:66:A:MET:HE1 | 1:42:A:TRP:HE1 | 19       | 0.15          |
| (1,1510) | 1:66:A:MET:HE2 | 1:42:A:TRP:HE1 | 19       | 0.15          |
| (1,1510) | 1:66:A:MET:HE3 | 1:42:A:TRP:HE1 | 19       | 0.15          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1510) | 1:66:A:MET:HE1 | 1:42:A:TRP:HE1 | 21       | 0.15          |
| (1,1510) | 1:66:A:MET:HE2 | 1:42:A:TRP:HE1 | 21       | 0.15          |
| (1,1510) | 1:66:A:MET:HE3 | 1:42:A:TRP:HE1 | 21       | 0.15          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 19       | 0.15          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 19       | 0.15          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 19       | 0.15          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 19       | 0.15          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 19       | 0.15          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 19       | 0.15          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 27       | 0.15          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 27       | 0.15          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 27       | 0.15          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 27       | 0.15          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 27       | 0.15          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 27       | 0.15          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 33       | 0.15          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 33       | 0.15          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 33       | 0.15          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 33       | 0.15          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 33       | 0.15          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 33       | 0.15          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 35       | 0.15          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 35       | 0.15          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 35       | 0.15          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 35       | 0.15          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 35       | 0.15          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 35       | 0.15          |
| (1,1508) | 1:66:A:MET:HE1 | 1:42:A:TRP:HZ3 | 20       | 0.15          |
| (1,1508) | 1:66:A:MET:HE2 | 1:42:A:TRP:HZ3 | 20       | 0.15          |
| (1,1508) | 1:66:A:MET:HE3 | 1:42:A:TRP:HZ3 | 20       | 0.15          |
| (1,1508) | 1:66:A:MET:HE1 | 1:42:A:TRP:HZ3 | 23       | 0.15          |
| (1,1508) | 1:66:A:MET:HE2 | 1:42:A:TRP:HZ3 | 23       | 0.15          |
| (1,1508) | 1:66:A:MET:HE3 | 1:42:A:TRP:HZ3 | 23       | 0.15          |
| (1,1508) | 1:66:A:MET:HE1 | 1:42:A:TRP:HZ3 | 25       | 0.15          |
| (1,1508) | 1:66:A:MET:HE2 | 1:42:A:TRP:HZ3 | 25       | 0.15          |
| (1,1508) | 1:66:A:MET:HE3 | 1:42:A:TRP:HZ3 | 25       | 0.15          |
| (1,1508) | 1:66:A:MET:HE1 | 1:42:A:TRP:HZ3 | 27       | 0.15          |
| (1,1508) | 1:66:A:MET:HE2 | 1:42:A:TRP:HZ3 | 27       | 0.15          |
| (1,1508) | 1:66:A:MET:HE3 | 1:42:A:TRP:HZ3 | 27       | 0.15          |
| (1,1508) | 1:66:A:MET:HE1 | 1:42:A:TRP:HZ3 | 38       | 0.15          |
| (1,1508) | 1:66:A:MET:HE2 | 1:42:A:TRP:HZ3 | 38       | 0.15          |
| (1,1508) | 1:66:A:MET:HE3 | 1:42:A:TRP:HZ3 | 38       | 0.15          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1500) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2 | 2        | 0.15          |
| (1,1500) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2 | 2        | 0.15          |
| (1,1500) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2 | 2        | 0.15          |
| (1,1500) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2 | 7        | 0.15          |
| (1,1500) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2 | 7        | 0.15          |
| (1,1500) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2 | 7        | 0.15          |
| (1,1500) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2 | 10       | 0.15          |
| (1,1500) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2 | 10       | 0.15          |
| (1,1500) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2 | 10       | 0.15          |
| (1,1500) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2 | 21       | 0.15          |
| (1,1500) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2 | 21       | 0.15          |
| (1,1500) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2 | 21       | 0.15          |
| (1,1500) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2 | 28       | 0.15          |
| (1,1500) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2 | 28       | 0.15          |
| (1,1500) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2 | 28       | 0.15          |
| (1,1494) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ  | 20       | 0.15          |
| (1,1494) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ  | 20       | 0.15          |
| (1,1494) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ  | 20       | 0.15          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 16       | 0.15          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 16       | 0.15          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 16       | 0.15          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA  | 27       | 0.15          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA  | 27       | 0.15          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 27       | 0.15          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H   | 5        | 0.15          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H   | 5        | 0.15          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H   | 5        | 0.15          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H   | 20       | 0.15          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H   | 20       | 0.15          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H   | 20       | 0.15          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H   | 28       | 0.15          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H   | 28       | 0.15          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H   | 28       | 0.15          |
| (1,1466) | 1:78:A:VAL:HG21 | 1:77:A:GLY:HA3 | 26       | 0.15          |
| (1,1466) | 1:78:A:VAL:HG22 | 1:77:A:GLY:HA3 | 26       | 0.15          |
| (1,1466) | 1:78:A:VAL:HG23 | 1:77:A:GLY:HA3 | 26       | 0.15          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 17       | 0.15          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 17       | 0.15          |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 17       | 0.15          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H   | 29       | 0.15          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H   | 29       | 0.15          |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H   | 29       | 0.15          |

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| Key      | Atom-1         | Atom-2       | Model ID | Violation (Å) |
|----------|----------------|--------------|----------|---------------|
| (1,1403) | 1:95:A:ALA:HB1 | 1:18:A:ASN:H | 11       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB2 | 1:18:A:ASN:H | 11       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB3 | 1:18:A:ASN:H | 11       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB1 | 1:18:A:ASN:H | 13       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB2 | 1:18:A:ASN:H | 13       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB3 | 1:18:A:ASN:H | 13       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB1 | 1:18:A:ASN:H | 15       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB2 | 1:18:A:ASN:H | 15       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB3 | 1:18:A:ASN:H | 15       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB1 | 1:18:A:ASN:H | 18       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB2 | 1:18:A:ASN:H | 18       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB3 | 1:18:A:ASN:H | 18       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB1 | 1:18:A:ASN:H | 19       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB2 | 1:18:A:ASN:H | 19       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB3 | 1:18:A:ASN:H | 19       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB1 | 1:18:A:ASN:H | 23       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB2 | 1:18:A:ASN:H | 23       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB3 | 1:18:A:ASN:H | 23       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB1 | 1:18:A:ASN:H | 33       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB2 | 1:18:A:ASN:H | 33       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB3 | 1:18:A:ASN:H | 33       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB1 | 1:18:A:ASN:H | 35       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB2 | 1:18:A:ASN:H | 35       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB3 | 1:18:A:ASN:H | 35       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB1 | 1:18:A:ASN:H | 36       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB2 | 1:18:A:ASN:H | 36       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB3 | 1:18:A:ASN:H | 36       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB1 | 1:18:A:ASN:H | 38       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB2 | 1:18:A:ASN:H | 38       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB3 | 1:18:A:ASN:H | 38       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB1 | 1:18:A:ASN:H | 40       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB2 | 1:18:A:ASN:H | 40       | 0.15          |
| (1,1403) | 1:95:A:ALA:HB3 | 1:18:A:ASN:H | 40       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H | 1        | 0.15          |
| (1,1401) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H | 1        | 0.15          |
| (1,1401) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H | 1        | 0.15          |
| (1,1401) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H | 4        | 0.15          |
| (1,1401) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H | 4        | 0.15          |
| (1,1401) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H | 4        | 0.15          |
| (1,1401) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H | 8        | 0.15          |
| (1,1401) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H | 8        | 0.15          |
| (1,1401) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H | 8        | 0.15          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1401) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H    | 10       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H    | 10       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 10       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H    | 12       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H    | 12       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 12       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H    | 16       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H    | 16       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 16       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H    | 18       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H    | 18       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 18       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H    | 20       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H    | 20       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 20       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H    | 23       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H    | 23       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 23       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H    | 24       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H    | 24       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 24       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H    | 25       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H    | 25       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 25       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H    | 30       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H    | 30       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 30       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H    | 32       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H    | 32       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 32       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H    | 34       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H    | 34       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 34       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H    | 35       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H    | 35       | 0.15          |
| (1,1401) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 35       | 0.15          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 1        | 0.15          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 1        | 0.15          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 1        | 0.15          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 9        | 0.15          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 9        | 0.15          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 9        | 0.15          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 12       | 0.15          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 12       | 0.15          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 12       | 0.15          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 23       | 0.15          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 23       | 0.15          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 23       | 0.15          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 29       | 0.15          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 29       | 0.15          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 29       | 0.15          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 36       | 0.15          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 36       | 0.15          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 36       | 0.15          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 37       | 0.15          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 37       | 0.15          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 37       | 0.15          |
| (1,1387) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ   | 9        | 0.15          |
| (1,1387) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ   | 9        | 0.15          |
| (1,1387) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ   | 9        | 0.15          |
| (1,1387) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ   | 15       | 0.15          |
| (1,1387) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ   | 15       | 0.15          |
| (1,1387) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ   | 15       | 0.15          |
| (1,1387) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ   | 33       | 0.15          |
| (1,1387) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ   | 33       | 0.15          |
| (1,1387) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ   | 33       | 0.15          |
| (1,1387) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ   | 34       | 0.15          |
| (1,1387) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ   | 34       | 0.15          |
| (1,1387) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ   | 34       | 0.15          |
| (1,1387) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ   | 37       | 0.15          |
| (1,1387) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ   | 37       | 0.15          |
| (1,1387) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ   | 37       | 0.15          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1  | 26       | 0.15          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2  | 26       | 0.15          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3  | 26       | 0.15          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1  | 26       | 0.15          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2  | 26       | 0.15          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3  | 26       | 0.15          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1  | 26       | 0.15          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2  | 26       | 0.15          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3  | 26       | 0.15          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1  | 37       | 0.15          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2  | 37       | 0.15          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3  | 37       | 0.15          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 37       | 0.15          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 37       | 0.15          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 37       | 0.15          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 37       | 0.15          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 37       | 0.15          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 37       | 0.15          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 38       | 0.15          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 38       | 0.15          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 38       | 0.15          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 38       | 0.15          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 38       | 0.15          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 38       | 0.15          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 38       | 0.15          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 38       | 0.15          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 38       | 0.15          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 26       | 0.15          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 26       | 0.15          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 26       | 0.15          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 26       | 0.15          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 26       | 0.15          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 26       | 0.15          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 26       | 0.15          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 26       | 0.15          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 26       | 0.15          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 37       | 0.15          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 37       | 0.15          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 37       | 0.15          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 37       | 0.15          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 37       | 0.15          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 37       | 0.15          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 37       | 0.15          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 37       | 0.15          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 37       | 0.15          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 38       | 0.15          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 38       | 0.15          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 38       | 0.15          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 38       | 0.15          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 38       | 0.15          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 38       | 0.15          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 38       | 0.15          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 38       | 0.15          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 38       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 3        | 0.15          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 19       | 0.15          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 21       | 0.15          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 32       | 0.15          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 2        | 0.15          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 16       | 0.15          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 17       | 0.15          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 22       | 0.15          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 28       | 0.15          |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 1        | 0.15          |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 24       | 0.15          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 1        | 0.15          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 1        | 0.15          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 1        | 0.15          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 4        | 0.15          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 4        | 0.15          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 4        | 0.15          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 6        | 0.15          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 6        | 0.15          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 6        | 0.15          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 10       | 0.15          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 10       | 0.15          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 10       | 0.15          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 13       | 0.15          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 13       | 0.15          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 13       | 0.15          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 23       | 0.15          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 23       | 0.15          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 23       | 0.15          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 27       | 0.15          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 27       | 0.15          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 27       | 0.15          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 34       | 0.15          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 34       | 0.15          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 34       | 0.15          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 39       | 0.15          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 39       | 0.15          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 39       | 0.15          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1  | 4        | 0.15          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2  | 4        | 0.15          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3  | 4        | 0.15          |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1  | 4        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2  | 4        | 0.15          |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3  | 4        | 0.15          |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1  | 4        | 0.15          |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2  | 4        | 0.15          |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3  | 4        | 0.15          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 1        | 0.15          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 1        | 0.15          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 1        | 0.15          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 4        | 0.15          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 4        | 0.15          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 4        | 0.15          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 6        | 0.15          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 6        | 0.15          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 6        | 0.15          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 10       | 0.15          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 10       | 0.15          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 10       | 0.15          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 13       | 0.15          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 13       | 0.15          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 13       | 0.15          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 23       | 0.15          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 23       | 0.15          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 23       | 0.15          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 27       | 0.15          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 27       | 0.15          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 27       | 0.15          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 34       | 0.15          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 34       | 0.15          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 34       | 0.15          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 39       | 0.15          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 39       | 0.15          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 39       | 0.15          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 5        | 0.15          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 5        | 0.15          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 5        | 0.15          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 5        | 0.15          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 5        | 0.15          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 5        | 0.15          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 5        | 0.15          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 5        | 0.15          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 5        | 0.15          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 6        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 6        | 0.15          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 6        | 0.15          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 6        | 0.15          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 6        | 0.15          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 6        | 0.15          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 6        | 0.15          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 6        | 0.15          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 6        | 0.15          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 7        | 0.15          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 7        | 0.15          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 7        | 0.15          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 7        | 0.15          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 7        | 0.15          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 7        | 0.15          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 7        | 0.15          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 7        | 0.15          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 7        | 0.15          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 9        | 0.15          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 9        | 0.15          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 9        | 0.15          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 9        | 0.15          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 9        | 0.15          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 9        | 0.15          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 9        | 0.15          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 9        | 0.15          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 9        | 0.15          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 11       | 0.15          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 11       | 0.15          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 11       | 0.15          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 11       | 0.15          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 11       | 0.15          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 11       | 0.15          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 11       | 0.15          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 11       | 0.15          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 11       | 0.15          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 25       | 0.15          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 25       | 0.15          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 25       | 0.15          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 25       | 0.15          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 25       | 0.15          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 25       | 0.15          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 25       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 25       | 0.15          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 25       | 0.15          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 31       | 0.15          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 31       | 0.15          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 31       | 0.15          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 31       | 0.15          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 31       | 0.15          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 31       | 0.15          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 31       | 0.15          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 31       | 0.15          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 31       | 0.15          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 36       | 0.15          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 36       | 0.15          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 36       | 0.15          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 36       | 0.15          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 36       | 0.15          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 36       | 0.15          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 36       | 0.15          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 36       | 0.15          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 36       | 0.15          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 7        | 0.15          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 7        | 0.15          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 7        | 0.15          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 14       | 0.15          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 14       | 0.15          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 14       | 0.15          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 19       | 0.15          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 19       | 0.15          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 19       | 0.15          |
| (1,1257) | 1:67:A:THR:HG21 | 1:26:A:SER:HB2  | 11       | 0.15          |
| (1,1257) | 1:67:A:THR:HG22 | 1:26:A:SER:HB2  | 11       | 0.15          |
| (1,1257) | 1:67:A:THR:HG23 | 1:26:A:SER:HB2  | 11       | 0.15          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 2        | 0.15          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 2        | 0.15          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 2        | 0.15          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 6        | 0.15          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 6        | 0.15          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 6        | 0.15          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 9        | 0.15          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 9        | 0.15          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 9        | 0.15          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 18       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 18       | 0.15          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 18       | 0.15          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 23       | 0.15          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 23       | 0.15          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 23       | 0.15          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 29       | 0.15          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 29       | 0.15          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 29       | 0.15          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 30       | 0.15          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 30       | 0.15          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 30       | 0.15          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 32       | 0.15          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 32       | 0.15          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 32       | 0.15          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 38       | 0.15          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 38       | 0.15          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 38       | 0.15          |
| (1,1239) | 1:13:A:THR:HG21 | 1:34:A:SER:H    | 14       | 0.15          |
| (1,1239) | 1:13:A:THR:HG22 | 1:34:A:SER:H    | 14       | 0.15          |
| (1,1239) | 1:13:A:THR:HG23 | 1:34:A:SER:H    | 14       | 0.15          |
| (1,1239) | 1:13:A:THR:HG21 | 1:34:A:SER:H    | 23       | 0.15          |
| (1,1239) | 1:13:A:THR:HG22 | 1:34:A:SER:H    | 23       | 0.15          |
| (1,1239) | 1:13:A:THR:HG23 | 1:34:A:SER:H    | 23       | 0.15          |
| (1,1239) | 1:13:A:THR:HG21 | 1:34:A:SER:H    | 36       | 0.15          |
| (1,1239) | 1:13:A:THR:HG22 | 1:34:A:SER:H    | 36       | 0.15          |
| (1,1239) | 1:13:A:THR:HG23 | 1:34:A:SER:H    | 36       | 0.15          |
| (1,1226) | 1:101:A:LEU:H   | 1:22:A:SER:HA   | 15       | 0.15          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 15       | 0.15          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 15       | 0.15          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 15       | 0.15          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 27       | 0.15          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 27       | 0.15          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 27       | 0.15          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG21 | 24       | 0.15          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG22 | 24       | 0.15          |
| (1,1200) | 1:39:A:ILE:H    | 1:39:A:ILE:HG23 | 24       | 0.15          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 4        | 0.15          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 4        | 0.15          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 4        | 0.15          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 10       | 0.15          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 10       | 0.15          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 10       | 0.15          |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1190) | 1:22:A:SER:H  | 1:21:A:VAL:HG21 | 11       | 0.15          |
| (1,1190) | 1:22:A:SER:H  | 1:21:A:VAL:HG22 | 11       | 0.15          |
| (1,1190) | 1:22:A:SER:H  | 1:21:A:VAL:HG23 | 11       | 0.15          |
| (1,1190) | 1:22:A:SER:H  | 1:21:A:VAL:HG21 | 14       | 0.15          |
| (1,1190) | 1:22:A:SER:H  | 1:21:A:VAL:HG22 | 14       | 0.15          |
| (1,1190) | 1:22:A:SER:H  | 1:21:A:VAL:HG23 | 14       | 0.15          |
| (1,1190) | 1:22:A:SER:H  | 1:21:A:VAL:HG21 | 16       | 0.15          |
| (1,1190) | 1:22:A:SER:H  | 1:21:A:VAL:HG22 | 16       | 0.15          |
| (1,1190) | 1:22:A:SER:H  | 1:21:A:VAL:HG23 | 16       | 0.15          |
| (1,1190) | 1:22:A:SER:H  | 1:21:A:VAL:HG21 | 17       | 0.15          |
| (1,1190) | 1:22:A:SER:H  | 1:21:A:VAL:HG22 | 17       | 0.15          |
| (1,1190) | 1:22:A:SER:H  | 1:21:A:VAL:HG23 | 17       | 0.15          |
| (1,1190) | 1:22:A:SER:H  | 1:21:A:VAL:HG21 | 22       | 0.15          |
| (1,1190) | 1:22:A:SER:H  | 1:21:A:VAL:HG22 | 22       | 0.15          |
| (1,1190) | 1:22:A:SER:H  | 1:21:A:VAL:HG23 | 22       | 0.15          |
| (1,1190) | 1:22:A:SER:H  | 1:21:A:VAL:HG21 | 40       | 0.15          |
| (1,1190) | 1:22:A:SER:H  | 1:21:A:VAL:HG22 | 40       | 0.15          |
| (1,1190) | 1:22:A:SER:H  | 1:21:A:VAL:HG23 | 40       | 0.15          |
| (1,1185) | 1:21:A:VAL:H  | 1:100:A:GLU:HB3 | 5        | 0.15          |
| (1,1177) | 1:100:A:GLU:H | 1:21:A:VAL:HG11 | 6        | 0.15          |
| (1,1177) | 1:100:A:GLU:H | 1:21:A:VAL:HG12 | 6        | 0.15          |
| (1,1177) | 1:100:A:GLU:H | 1:21:A:VAL:HG13 | 6        | 0.15          |
| (1,1174) | 1:91:A:ALA:H  | 1:84:A:ARG:HA   | 5        | 0.15          |
| (1,1163) | 1:75:A:ASP:H  | 1:74:A:ASP:HB2  | 11       | 0.15          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 7        | 0.15          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 7        | 0.15          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 9        | 0.15          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 9        | 0.15          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 18       | 0.15          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 18       | 0.15          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 26       | 0.15          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 26       | 0.15          |
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 6        | 0.15          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 22       | 0.15          |
| (1,1052) | 1:26:A:SER:H  | 1:25:A:GLN:HG2  | 20       | 0.15          |
| (1,1052) | 1:26:A:SER:H  | 1:25:A:GLN:HG2  | 29       | 0.15          |
| (1,1020) | 1:48:A:GLU:H  | 1:48:A:GLU:HG3  | 6        | 0.15          |
| (1,1020) | 1:48:A:GLU:H  | 1:48:A:GLU:HG3  | 11       | 0.15          |
| (1,1020) | 1:48:A:GLU:H  | 1:48:A:GLU:HG3  | 29       | 0.15          |
| (1,1002) | 1:5:A:PHE:H   | 1:4:A:PRO:HA    | 15       | 0.15          |
| (1,1002) | 1:5:A:PHE:H   | 1:4:A:PRO:HA    | 18       | 0.15          |
| (1,997)  | 1:79:A:TYR:H  | 1:94:A:THR:HG21 | 2        | 0.15          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,997) | 1:79:A:TYR:H | 1:94:A:THR:HG22 | 2        | 0.15          |
| (1,997) | 1:79:A:TYR:H | 1:94:A:THR:HG23 | 2        | 0.15          |
| (1,997) | 1:79:A:TYR:H | 1:94:A:THR:HG21 | 19       | 0.15          |
| (1,997) | 1:79:A:TYR:H | 1:94:A:THR:HG22 | 19       | 0.15          |
| (1,997) | 1:79:A:TYR:H | 1:94:A:THR:HG23 | 19       | 0.15          |
| (1,987) | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 16       | 0.15          |
| (1,987) | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 18       | 0.15          |
| (1,987) | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 22       | 0.15          |
| (1,987) | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 24       | 0.15          |
| (1,987) | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 25       | 0.15          |
| (1,987) | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 28       | 0.15          |
| (1,987) | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 30       | 0.15          |
| (1,987) | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 32       | 0.15          |
| (1,987) | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 35       | 0.15          |
| (1,987) | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 37       | 0.15          |
| (1,987) | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 40       | 0.15          |
| (1,978) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 2        | 0.15          |
| (1,978) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 16       | 0.15          |
| (1,978) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 17       | 0.15          |
| (1,978) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 22       | 0.15          |
| (1,978) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 28       | 0.15          |
| (1,971) | 1:21:A:VAL:H | 1:21:A:VAL:HG21 | 5        | 0.15          |
| (1,971) | 1:21:A:VAL:H | 1:21:A:VAL:HG22 | 5        | 0.15          |
| (1,971) | 1:21:A:VAL:H | 1:21:A:VAL:HG23 | 5        | 0.15          |
| (1,967) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 3        | 0.15          |
| (1,967) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 12       | 0.15          |
| (1,967) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 18       | 0.15          |
| (1,967) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 29       | 0.15          |
| (1,967) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 37       | 0.15          |
| (1,967) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 38       | 0.15          |
| (1,967) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 39       | 0.15          |
| (1,941) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 3        | 0.15          |
| (1,941) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 31       | 0.15          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 2        | 0.15          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 2        | 0.15          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 2        | 0.15          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 4        | 0.15          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 4        | 0.15          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 4        | 0.15          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 10       | 0.15          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 10       | 0.15          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 10       | 0.15          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 12       | 0.15          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 12       | 0.15          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 12       | 0.15          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 15       | 0.15          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 15       | 0.15          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 15       | 0.15          |
| (1,899) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 20       | 0.15          |
| (1,888) | 1:80:A:SER:H | 1:43:A:TYR:HB3  | 1        | 0.15          |
| (1,888) | 1:80:A:SER:H | 1:43:A:TYR:HB3  | 5        | 0.15          |
| (1,888) | 1:80:A:SER:H | 1:43:A:TYR:HB3  | 30       | 0.15          |
| (1,875) | 1:8:A:GLU:H  | 1:7:A:ALA:HB1   | 16       | 0.15          |
| (1,875) | 1:8:A:GLU:H  | 1:7:A:ALA:HB2   | 16       | 0.15          |
| (1,875) | 1:8:A:GLU:H  | 1:7:A:ALA:HB3   | 16       | 0.15          |
| (1,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3   | 2        | 0.15          |
| (1,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3   | 8        | 0.15          |
| (1,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 22       | 0.15          |
| (1,869) | 1:8:A:GLU:H  | 1:7:A:ALA:HA    | 35       | 0.15          |
| (1,863) | 1:86:A:GLU:H | 1:85:A:LEU:HB3  | 33       | 0.15          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 22       | 0.15          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 22       | 0.15          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 22       | 0.15          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 30       | 0.15          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 30       | 0.15          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 30       | 0.15          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 32       | 0.15          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 32       | 0.15          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 32       | 0.15          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 5        | 0.15          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 5        | 0.15          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 5        | 0.15          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 29       | 0.15          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 29       | 0.15          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 29       | 0.15          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 39       | 0.15          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 39       | 0.15          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 39       | 0.15          |
| (1,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB   | 20       | 0.15          |
| (1,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB   | 22       | 0.15          |
| (1,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB   | 23       | 0.15          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 5        | 0.15          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 5        | 0.15          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 5        | 0.15          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG11 | 20       | 0.15          |
| (1,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG12 | 20       | 0.15          |
| (1,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG13 | 20       | 0.15          |
| (1,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG11 | 28       | 0.15          |
| (1,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG12 | 28       | 0.15          |
| (1,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG13 | 28       | 0.15          |
| (1,801) | 1:54:A:LYS:H  | 1:54:A:LYS:HD2  | 19       | 0.15          |
| (1,801) | 1:54:A:LYS:H  | 1:54:A:LYS:HD2  | 28       | 0.15          |
| (1,786) | 1:6:A:THR:H   | 1:6:A:THR:HG21  | 29       | 0.15          |
| (1,786) | 1:6:A:THR:H   | 1:6:A:THR:HG22  | 29       | 0.15          |
| (1,786) | 1:6:A:THR:H   | 1:6:A:THR:HG23  | 29       | 0.15          |
| (1,776) | 1:6:A:THR:H   | 1:6:A:THR:HA    | 16       | 0.15          |
| (1,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 22       | 0.15          |
| (1,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 27       | 0.15          |
| (1,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 30       | 0.15          |
| (1,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 38       | 0.15          |
| (1,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 7        | 0.15          |
| (1,672) | 1:72:A:THR:H  | 1:73:A:PRO:HD2  | 18       | 0.15          |
| (1,661) | 1:7:A:ALA:H   | 1:6:A:THR:HA    | 8        | 0.15          |
| (1,661) | 1:7:A:ALA:H   | 1:6:A:THR:HA    | 23       | 0.15          |
| (1,661) | 1:7:A:ALA:H   | 1:6:A:THR:HA    | 36       | 0.15          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 9        | 0.15          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 16       | 0.15          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 24       | 0.15          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 34       | 0.15          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 39       | 0.15          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 40       | 0.15          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 24       | 0.15          |
| (1,605) | 1:50:A:THR:H  | 1:49:A:LEU:HB2  | 37       | 0.15          |
| (1,591) | 1:3:A:ASP:H   | 1:3:A:ASP:HA    | 40       | 0.15          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 2        | 0.15          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 2        | 0.15          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 2        | 0.15          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 11       | 0.15          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 11       | 0.15          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 11       | 0.15          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 21       | 0.15          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 21       | 0.15          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 21       | 0.15          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 22       | 0.15          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 22       | 0.15          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 22       | 0.15          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 23       | 0.15          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 23       | 0.15          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 23       | 0.15          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 25       | 0.15          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 25       | 0.15          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 25       | 0.15          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 30       | 0.15          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 30       | 0.15          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 30       | 0.15          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 34       | 0.15          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 34       | 0.15          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 34       | 0.15          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 36       | 0.15          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 36       | 0.15          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 36       | 0.15          |
| (1,560) | 1:47:A:THR:H | 1:47:A:THR:HA   | 18       | 0.15          |
| (1,560) | 1:47:A:THR:H | 1:47:A:THR:HA   | 19       | 0.15          |
| (1,560) | 1:47:A:THR:H | 1:47:A:THR:HA   | 31       | 0.15          |
| (1,560) | 1:47:A:THR:H | 1:47:A:THR:HA   | 33       | 0.15          |
| (1,560) | 1:47:A:THR:H | 1:47:A:THR:HA   | 39       | 0.15          |
| (1,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1  | 7        | 0.15          |
| (1,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2  | 7        | 0.15          |
| (1,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1  | 19       | 0.15          |
| (1,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2  | 19       | 0.15          |
| (1,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 8        | 0.15          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 6        | 0.15          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 12       | 0.15          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 14       | 0.15          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 37       | 0.15          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 13       | 0.15          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 29       | 0.15          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 31       | 0.15          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 3        | 0.15          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 4        | 0.15          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 6        | 0.15          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 11       | 0.15          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 13       | 0.15          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 19       | 0.15          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 21       | 0.15          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 23       | 0.15          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 25       | 0.15          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 31       | 0.15          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 33       | 0.15          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 35       | 0.15          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 36       | 0.15          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 37       | 0.15          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 39       | 0.15          |
| (1,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 5        | 0.15          |
| (1,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 8        | 0.15          |
| (1,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 15       | 0.15          |
| (1,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 37       | 0.15          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 1        | 0.15          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 2        | 0.15          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 10       | 0.15          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 11       | 0.15          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 18       | 0.15          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 21       | 0.15          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 24       | 0.15          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 31       | 0.15          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 32       | 0.15          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 33       | 0.15          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 34       | 0.15          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 40       | 0.15          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 2        | 0.15          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 5        | 0.15          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 12       | 0.15          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 16       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 3        | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 3        | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 3        | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 4        | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 4        | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 4        | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 9        | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 9        | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 9        | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 11       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 11       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 11       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 15       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 15       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 15       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 16       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 16       | 0.15          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 16       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 20       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 20       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 20       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 22       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 22       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 22       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 23       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 23       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 23       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 25       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 25       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 25       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 26       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 26       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 26       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 28       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 28       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 28       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 32       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 32       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 32       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 36       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 36       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 36       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 37       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 37       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 37       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 38       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 38       | 0.15          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 38       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 11       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 11       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 11       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 13       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 13       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 13       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 15       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 15       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 15       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 18       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 18       | 0.15          |

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| Key     | Atom-1       | Atom-2         | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3 | 18       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1 | 19       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2 | 19       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3 | 19       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1 | 23       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2 | 23       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3 | 23       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1 | 33       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2 | 33       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3 | 33       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1 | 35       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2 | 35       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3 | 35       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1 | 36       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2 | 36       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3 | 36       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1 | 38       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2 | 38       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3 | 38       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1 | 40       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2 | 40       | 0.15          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3 | 40       | 0.15          |
| (1,368) | 1:18:A:ASN:H | 1:17:A:GLN:HB3 | 5        | 0.15          |
| (1,343) | 1:14:A:LYS:H | 1:33:A:VAL:HA  | 20       | 0.15          |
| (1,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD1 | 12       | 0.15          |
| (1,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD2 | 12       | 0.15          |
| (1,314) | 1:63:A:CYS:H | 1:64:A:HIS:HD2 | 27       | 0.15          |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3 | 9        | 0.15          |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3 | 15       | 0.15          |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3 | 20       | 0.15          |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3 | 23       | 0.15          |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3 | 26       | 0.15          |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3 | 32       | 0.15          |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3 | 34       | 0.15          |
| (1,274) | 1:66:A:MET:H | 1:66:A:MET:HG3 | 4        | 0.15          |
| (1,242) | 1:95:A:ALA:H | 1:96:A:GLU:H   | 28       | 0.15          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1 | 6        | 0.15          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2 | 6        | 0.15          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1 | 9        | 0.15          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2 | 9        | 0.15          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1 | 20       | 0.15          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2 | 20       | 0.15          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 3        | 0.15          |
| (1,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 5        | 0.15          |
| (1,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 8        | 0.15          |
| (1,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 10       | 0.15          |
| (1,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 12       | 0.15          |
| (1,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 20       | 0.15          |
| (1,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 27       | 0.15          |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG21 | 3        | 0.15          |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG22 | 3        | 0.15          |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG23 | 3        | 0.15          |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG21 | 32       | 0.15          |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG22 | 32       | 0.15          |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG23 | 32       | 0.15          |
| (1,198) | 1:90:A:GLU:H  | 1:90:A:GLU:HB2  | 27       | 0.15          |
| (1,198) | 1:90:A:GLU:H  | 1:90:A:GLU:HB2  | 28       | 0.15          |
| (1,198) | 1:90:A:GLU:H  | 1:90:A:GLU:HB2  | 30       | 0.15          |
| (1,198) | 1:90:A:GLU:H  | 1:90:A:GLU:HB2  | 34       | 0.15          |
| (1,148) | 1:45:A:GLY:H  | 1:46:A:PRO:HD2  | 28       | 0.15          |
| (1,148) | 1:45:A:GLY:H  | 1:46:A:PRO:HD2  | 30       | 0.15          |
| (1,148) | 1:45:A:GLY:H  | 1:46:A:PRO:HD2  | 32       | 0.15          |
| (1,148) | 1:45:A:GLY:H  | 1:46:A:PRO:HD2  | 38       | 0.15          |
| (1,148) | 1:45:A:GLY:H  | 1:46:A:PRO:HD2  | 39       | 0.15          |
| (1,142) | 1:101:A:LEU:H | 1:100:A:GLU:HB2 | 14       | 0.15          |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 6        | 0.15          |
| (1,111) | 1:63:A:CYS:H  | 1:60:A:ASP:H    | 16       | 0.15          |
| (1,100) | 1:22:A:SER:H  | 1:21:A:VAL:HB   | 3        | 0.15          |
| (1,70)  | 1:51:A:GLU:H  | 1:51:A:GLU:HG2  | 15       | 0.15          |
| (1,57)  | 1:42:A:TRP:H  | 1:41:A:THR:HB   | 4        | 0.15          |
| (1,57)  | 1:42:A:TRP:H  | 1:41:A:THR:HB   | 6        | 0.15          |
| (1,57)  | 1:42:A:TRP:H  | 1:41:A:THR:HB   | 22       | 0.15          |
| (1,57)  | 1:42:A:TRP:H  | 1:41:A:THR:HB   | 33       | 0.15          |
| (1,49)  | 1:57:A:PHE:H  | 1:56:A:ASN:HB2  | 20       | 0.15          |
| (1,49)  | 1:57:A:PHE:H  | 1:56:A:ASN:HB2  | 34       | 0.15          |
| (1,49)  | 1:57:A:PHE:H  | 1:56:A:ASN:HB2  | 36       | 0.15          |
| (1,48)  | 1:57:A:PHE:H  | 1:57:A:PHE:HB3  | 1        | 0.15          |
| (1,48)  | 1:57:A:PHE:H  | 1:57:A:PHE:HB3  | 9        | 0.15          |
| (1,48)  | 1:57:A:PHE:H  | 1:57:A:PHE:HB3  | 13       | 0.15          |
| (1,48)  | 1:57:A:PHE:H  | 1:57:A:PHE:HB3  | 15       | 0.15          |
| (1,48)  | 1:57:A:PHE:H  | 1:57:A:PHE:HB3  | 18       | 0.15          |
| (1,48)  | 1:57:A:PHE:H  | 1:57:A:PHE:HB3  | 22       | 0.15          |
| (1,48)  | 1:57:A:PHE:H  | 1:57:A:PHE:HB3  | 23       | 0.15          |
| (1,48)  | 1:57:A:PHE:H  | 1:57:A:PHE:HB3  | 30       | 0.15          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 38       | 0.15          |
| (1,35)   | 1:88:A:ARG:H   | 1:88:A:ARG:HG2  | 10       | 0.15          |
| (1,35)   | 1:88:A:ARG:H   | 1:88:A:ARG:HG2  | 17       | 0.15          |
| (1,22)   | 1:89:A:GLY:H   | 1:85:A:LEU:H    | 8        | 0.15          |
| (1,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 6        | 0.15          |
| (1,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 11       | 0.15          |
| (1,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 15       | 0.15          |
| (1,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 18       | 0.15          |
| (1,18)   | 1:89:A:GLY:H   | 1:89:A:GLY:HA3  | 19       | 0.15          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 4        | 0.14          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 4        | 0.14          |
| (3,3218) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 10       | 0.14          |
| (3,3218) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 10       | 0.14          |
| (3,3217) | 1:69:A:HIS:HE1 | 1:67:A:THR:HB   | 30       | 0.14          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 21       | 0.14          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 21       | 0.14          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 21       | 0.14          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 21       | 0.14          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 21       | 0.14          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 21       | 0.14          |
| (3,3203) | 1:42:A:TRP:HZ2 | 1:30:A:GLU:HA   | 12       | 0.14          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 5        | 0.14          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 5        | 0.14          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 5        | 0.14          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 5        | 0.14          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 8        | 0.14          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 8        | 0.14          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 8        | 0.14          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 8        | 0.14          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 33       | 0.14          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 33       | 0.14          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 33       | 0.14          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 33       | 0.14          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 15       | 0.14          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 36       | 0.14          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 16       | 0.14          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 16       | 0.14          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 16       | 0.14          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 28       | 0.14          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 28       | 0.14          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 28       | 0.14          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 33       | 0.14          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2 | 33       | 0.14          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3 | 33       | 0.14          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1 | 39       | 0.14          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2 | 39       | 0.14          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3 | 39       | 0.14          |
| (3,3175) | 1:69:A:HIS:HD2 | 1:69:A:HIS:HB3 | 15       | 0.14          |
| (3,3175) | 1:69:A:HIS:HD2 | 1:69:A:HIS:HB3 | 17       | 0.14          |
| (3,3175) | 1:69:A:HIS:HD2 | 1:69:A:HIS:HB3 | 28       | 0.14          |
| (3,3175) | 1:69:A:HIS:HD2 | 1:69:A:HIS:HB3 | 29       | 0.14          |
| (3,3164) | 1:42:A:TRP:HD1 | 1:41:A:THR:HA  | 6        | 0.14          |
| (3,3164) | 1:42:A:TRP:HD1 | 1:41:A:THR:HA  | 11       | 0.14          |
| (3,3143) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3 | 7        | 0.14          |
| (3,3143) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3 | 7        | 0.14          |
| (3,3143) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3 | 15       | 0.14          |
| (3,3143) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3 | 15       | 0.14          |
| (3,3143) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3 | 16       | 0.14          |
| (3,3143) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3 | 16       | 0.14          |
| (3,3143) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3 | 20       | 0.14          |
| (3,3143) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3 | 20       | 0.14          |
| (3,3143) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3 | 35       | 0.14          |
| (3,3143) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3 | 35       | 0.14          |
| (3,3143) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3 | 36       | 0.14          |
| (3,3143) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3 | 36       | 0.14          |
| (3,3143) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3 | 39       | 0.14          |
| (3,3143) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3 | 39       | 0.14          |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 7        | 0.14          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 7        | 0.14          |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 10       | 0.14          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 10       | 0.14          |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 21       | 0.14          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 21       | 0.14          |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 24       | 0.14          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 24       | 0.14          |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 33       | 0.14          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 33       | 0.14          |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 37       | 0.14          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 37       | 0.14          |
| (3,3139) | 1:65:A:TYR:HE1 | 1:60:A:ASP:HB3 | 13       | 0.14          |
| (3,3139) | 1:65:A:TYR:HE2 | 1:60:A:ASP:HB3 | 13       | 0.14          |
| (3,3138) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB2 | 23       | 0.14          |
| (3,3138) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB2 | 23       | 0.14          |
| (3,3137) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3 | 15       | 0.14          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3137) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3  | 15       | 0.14          |
| (3,3137) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3  | 32       | 0.14          |
| (3,3137) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3  | 32       | 0.14          |
| (3,3137) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3  | 39       | 0.14          |
| (3,3137) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3  | 39       | 0.14          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 1        | 0.14          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 1        | 0.14          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 7        | 0.14          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 7        | 0.14          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 22       | 0.14          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 22       | 0.14          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 27       | 0.14          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 27       | 0.14          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 1        | 0.14          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 1        | 0.14          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 7        | 0.14          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 7        | 0.14          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 22       | 0.14          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 22       | 0.14          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 27       | 0.14          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 27       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 3        | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 3        | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 3        | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 3        | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 3        | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 3        | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 11       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 11       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 11       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 11       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 11       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 11       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 14       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 14       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 14       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 14       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 14       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 14       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 15       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 15       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 15       | 0.14          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 15       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 15       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 15       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 21       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 21       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 21       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 21       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 21       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 21       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 22       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 22       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 22       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 22       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 22       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 22       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 23       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 23       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 23       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 23       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 23       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 23       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 25       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 25       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 25       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 25       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 25       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 25       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 27       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 27       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 27       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 27       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 27       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 27       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 30       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 30       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 30       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 30       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 30       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 30       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 38       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 38       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 38       | 0.14          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 38       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 38       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 38       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 39       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 39       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 39       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 39       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 39       | 0.14          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 39       | 0.14          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 23       | 0.14          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 23       | 0.14          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 23       | 0.14          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 23       | 0.14          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 23       | 0.14          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 23       | 0.14          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 34       | 0.14          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 34       | 0.14          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 34       | 0.14          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 34       | 0.14          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 34       | 0.14          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 34       | 0.14          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 19       | 0.14          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 19       | 0.14          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 19       | 0.14          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 19       | 0.14          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 25       | 0.14          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 25       | 0.14          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 25       | 0.14          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 25       | 0.14          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 31       | 0.14          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 31       | 0.14          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 31       | 0.14          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 31       | 0.14          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 4        | 0.14          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 4        | 0.14          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 4        | 0.14          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 4        | 0.14          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 4        | 0.14          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 4        | 0.14          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 8        | 0.14          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 8        | 0.14          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 8        | 0.14          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 8        | 0.14          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 8        | 0.14          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 8        | 0.14          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 31       | 0.14          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 31       | 0.14          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 31       | 0.14          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 31       | 0.14          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 31       | 0.14          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 31       | 0.14          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 33       | 0.14          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 33       | 0.14          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 33       | 0.14          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 33       | 0.14          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 33       | 0.14          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 33       | 0.14          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 40       | 0.14          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 40       | 0.14          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 40       | 0.14          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 40       | 0.14          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 40       | 0.14          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 40       | 0.14          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 1        | 0.14          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 1        | 0.14          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 1        | 0.14          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 2        | 0.14          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 2        | 0.14          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 2        | 0.14          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 7        | 0.14          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 7        | 0.14          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 7        | 0.14          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 15       | 0.14          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 15       | 0.14          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 15       | 0.14          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 32       | 0.14          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 32       | 0.14          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 32       | 0.14          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 34       | 0.14          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 34       | 0.14          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 34       | 0.14          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 37       | 0.14          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 37       | 0.14          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 37       | 0.14          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 40       | 0.14          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 40       | 0.14          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 40       | 0.14          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 11       | 0.14          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 11       | 0.14          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 12       | 0.14          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 12       | 0.14          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 21       | 0.14          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 21       | 0.14          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 23       | 0.14          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 23       | 0.14          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 25       | 0.14          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 25       | 0.14          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 34       | 0.14          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 34       | 0.14          |
| (3,3055) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 9        | 0.14          |
| (3,3048) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG21 | 15       | 0.14          |
| (3,3048) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG22 | 15       | 0.14          |
| (3,3048) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG23 | 15       | 0.14          |
| (3,3041) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE1  | 4        | 0.14          |
| (3,3041) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE2  | 4        | 0.14          |
| (3,3041) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE1  | 9        | 0.14          |
| (3,3041) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE2  | 9        | 0.14          |
| (3,3041) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE1  | 39       | 0.14          |
| (3,3041) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE2  | 39       | 0.14          |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 1        | 0.14          |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 1        | 0.14          |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 19       | 0.14          |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 19       | 0.14          |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 28       | 0.14          |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 28       | 0.14          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 5        | 0.14          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 5        | 0.14          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 5        | 0.14          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 7        | 0.14          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 7        | 0.14          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 7        | 0.14          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 26       | 0.14          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 26       | 0.14          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 26       | 0.14          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 32       | 0.14          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 32       | 0.14          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 32       | 0.14          |
| (3,3019) | 1:30:A:GLU:HB2 | 1:14:A:LYS:HE2  | 4        | 0.14          |
| (3,3019) | 1:30:A:GLU:HB2 | 1:14:A:LYS:HE2  | 24       | 0.14          |
| (3,3019) | 1:30:A:GLU:HB2 | 1:14:A:LYS:HE2  | 28       | 0.14          |
| (3,3019) | 1:30:A:GLU:HB2 | 1:14:A:LYS:HE2  | 33       | 0.14          |
| (3,3004) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 5        | 0.14          |
| (3,3004) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 39       | 0.14          |
| (3,3004) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3  | 40       | 0.14          |
| (3,2982) | 1:65:A:TYR:HA  | 1:42:A:TRP:HZ2  | 28       | 0.14          |
| (3,2970) | 1:44:A:LYS:HE2 | 1:44:A:LYS:HG3  | 2        | 0.14          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2  | 15       | 0.14          |
| (3,2957) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA    | 6        | 0.14          |
| (3,2957) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA    | 15       | 0.14          |
| (3,2957) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA    | 26       | 0.14          |
| (3,2957) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA    | 29       | 0.14          |
| (3,2957) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA    | 30       | 0.14          |
| (3,2957) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA    | 36       | 0.14          |
| (3,2949) | 1:90:A:GLU:HA  | 1:84:A:ARG:HA   | 1        | 0.14          |
| (3,2949) | 1:90:A:GLU:HA  | 1:84:A:ARG:HA   | 5        | 0.14          |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1  | 7        | 0.14          |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2  | 7        | 0.14          |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1  | 15       | 0.14          |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2  | 15       | 0.14          |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1  | 16       | 0.14          |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2  | 16       | 0.14          |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1  | 20       | 0.14          |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2  | 20       | 0.14          |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1  | 35       | 0.14          |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2  | 35       | 0.14          |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1  | 36       | 0.14          |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2  | 36       | 0.14          |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1  | 39       | 0.14          |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2  | 39       | 0.14          |
| (3,2938) | 1:26:A:SER:HA  | 1:70:A:ASN:H    | 11       | 0.14          |
| (3,2938) | 1:26:A:SER:HA  | 1:70:A:ASN:H    | 30       | 0.14          |
| (3,2936) | 1:17:A:GLN:HG2 | 1:17:A:GLN:H    | 37       | 0.14          |
| (3,2910) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD2  | 1        | 0.14          |
| (3,2910) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD2  | 6        | 0.14          |
| (3,2910) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD2  | 8        | 0.14          |
| (3,2910) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD2  | 9        | 0.14          |
| (3,2910) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD2  | 19       | 0.14          |
| (3,2910) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD2  | 23       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 24       | 0.14          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 25       | 0.14          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 26       | 0.14          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 30       | 0.14          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 31       | 0.14          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 32       | 0.14          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 33       | 0.14          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 34       | 0.14          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 35       | 0.14          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 37       | 0.14          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 39       | 0.14          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 40       | 0.14          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 14       | 0.14          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 17       | 0.14          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 18       | 0.14          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 34       | 0.14          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 35       | 0.14          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 39       | 0.14          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 40       | 0.14          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 7        | 0.14          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 2        | 0.14          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 4        | 0.14          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 6        | 0.14          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 11       | 0.14          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 29       | 0.14          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 31       | 0.14          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 33       | 0.14          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 34       | 0.14          |
| (3,2761) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 4        | 0.14          |
| (3,2761) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 19       | 0.14          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H    | 3        | 0.14          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H    | 4        | 0.14          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H    | 6        | 0.14          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H    | 7        | 0.14          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H    | 12       | 0.14          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H    | 16       | 0.14          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H    | 19       | 0.14          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H    | 37       | 0.14          |
| (3,2719) | 1:48:A:GLU:HA   | 1:49:A:LEU:HG   | 16       | 0.14          |
| (3,2703) | 1:23:A:GLU:HA   | 1:24:A:HIS:HA   | 6        | 0.14          |
| (3,2690) | 1:8:A:GLU:HB3   | 1:8:A:GLU:HG2   | 6        | 0.14          |
| (3,2690) | 1:8:A:GLU:HB3   | 1:8:A:GLU:HG2   | 10       | 0.14          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2  | 20       | 0.14          |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2  | 26       | 0.14          |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2  | 30       | 0.14          |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2  | 33       | 0.14          |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2  | 34       | 0.14          |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2  | 36       | 0.14          |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2  | 37       | 0.14          |
| (3,2679) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 2        | 0.14          |
| (3,2679) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 8        | 0.14          |
| (3,2679) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 15       | 0.14          |
| (3,2679) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 18       | 0.14          |
| (3,2679) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 20       | 0.14          |
| (3,2679) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 23       | 0.14          |
| (3,2679) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 24       | 0.14          |
| (3,2679) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 27       | 0.14          |
| (3,2679) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 31       | 0.14          |
| (3,2679) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 32       | 0.14          |
| (3,2679) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 37       | 0.14          |
| (3,2679) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 40       | 0.14          |
| (3,2653) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H   | 1        | 0.14          |
| (3,2601) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 36       | 0.14          |
| (3,2554) | 1:92:A:ARG:HA  | 1:83:A:ALA:H   | 19       | 0.14          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 4        | 0.14          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 6        | 0.14          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 7        | 0.14          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 15       | 0.14          |
| (3,2541) | 1:73:A:PRO:HG3 | 1:73:A:PRO:HA  | 24       | 0.14          |
| (3,2541) | 1:73:A:PRO:HG3 | 1:73:A:PRO:HA  | 36       | 0.14          |
| (3,2541) | 1:73:A:PRO:HG3 | 1:73:A:PRO:HA  | 40       | 0.14          |
| (3,2514) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 14       | 0.14          |
| (3,2514) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 16       | 0.14          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2  | 8        | 0.14          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2  | 17       | 0.14          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA   | 3        | 0.14          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA   | 5        | 0.14          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA   | 6        | 0.14          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA   | 7        | 0.14          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA   | 12       | 0.14          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA   | 14       | 0.14          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA   | 28       | 0.14          |
| (3,2434) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 16       | 0.14          |
| (3,2434) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 27       | 0.14          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,2434) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 38       | 0.14          |
| (3,2419) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA   | 19       | 0.14          |
| (3,2419) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA   | 21       | 0.14          |
| (3,2419) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA   | 24       | 0.14          |
| (3,2419) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA   | 25       | 0.14          |
| (3,2419) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA   | 35       | 0.14          |
| (3,2412) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 1        | 0.14          |
| (3,2412) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 7        | 0.14          |
| (3,2412) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 10       | 0.14          |
| (3,2412) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 26       | 0.14          |
| (3,2412) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 27       | 0.14          |
| (3,2412) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 34       | 0.14          |
| (3,2406) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 5        | 0.14          |
| (3,2406) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 5        | 0.14          |
| (3,2406) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 5        | 0.14          |
| (3,2406) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 15       | 0.14          |
| (3,2406) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 15       | 0.14          |
| (3,2406) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 15       | 0.14          |
| (3,2406) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 31       | 0.14          |
| (3,2406) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 31       | 0.14          |
| (3,2406) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 31       | 0.14          |
| (3,2406) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 35       | 0.14          |
| (3,2406) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 35       | 0.14          |
| (3,2406) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 35       | 0.14          |
| (3,2406) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 37       | 0.14          |
| (3,2406) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 37       | 0.14          |
| (3,2406) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 37       | 0.14          |
| (3,2406) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 38       | 0.14          |
| (3,2406) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 38       | 0.14          |
| (3,2406) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 38       | 0.14          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 1        | 0.14          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 1        | 0.14          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 1        | 0.14          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 16       | 0.14          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 16       | 0.14          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 16       | 0.14          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 19       | 0.14          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 19       | 0.14          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 19       | 0.14          |
| (3,2290) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H   | 1        | 0.14          |
| (3,2290) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H   | 10       | 0.14          |
| (3,2290) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H   | 11       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2290) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 15       | 0.14          |
| (3,2290) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 20       | 0.14          |
| (3,2290) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 21       | 0.14          |
| (3,2290) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 23       | 0.14          |
| (3,2290) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 24       | 0.14          |
| (3,2290) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 26       | 0.14          |
| (3,2290) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 27       | 0.14          |
| (3,2290) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 30       | 0.14          |
| (3,2290) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 32       | 0.14          |
| (3,2290) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 36       | 0.14          |
| (3,2290) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 39       | 0.14          |
| (3,2290) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 40       | 0.14          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG21 | 11       | 0.14          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG22 | 11       | 0.14          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG23 | 11       | 0.14          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG21 | 34       | 0.14          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG22 | 34       | 0.14          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG23 | 34       | 0.14          |
| (3,2240) | 1:18:A:ASN:HB2  | 1:18:A:ASN:H    | 7        | 0.14          |
| (3,2240) | 1:18:A:ASN:HB2  | 1:18:A:ASN:H    | 22       | 0.14          |
| (3,2240) | 1:18:A:ASN:HB2  | 1:18:A:ASN:H    | 23       | 0.14          |
| (3,2240) | 1:18:A:ASN:HB2  | 1:18:A:ASN:H    | 31       | 0.14          |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD11 | 27       | 0.14          |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD12 | 27       | 0.14          |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD13 | 27       | 0.14          |
| (3,2148) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 13       | 0.14          |
| (3,2148) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 19       | 0.14          |
| (3,2148) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 34       | 0.14          |
| (3,2148) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 39       | 0.14          |
| (3,2139) | 1:67:A:THR:HB   | 1:56:A:ASN:HB2  | 4        | 0.14          |
| (3,2102) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HA   | 11       | 0.14          |
| (3,2102) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HA   | 11       | 0.14          |
| (3,2102) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HA   | 11       | 0.14          |
| (3,2102) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HA   | 22       | 0.14          |
| (3,2102) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HA   | 22       | 0.14          |
| (3,2102) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HA   | 22       | 0.14          |
| (3,2102) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HA   | 31       | 0.14          |
| (3,2102) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HA   | 31       | 0.14          |
| (3,2102) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HA   | 31       | 0.14          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 2        | 0.14          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 2        | 0.14          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 2        | 0.14          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2 | 16       | 0.14          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2 | 16       | 0.14          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2 | 16       | 0.14          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2 | 28       | 0.14          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2 | 28       | 0.14          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2 | 28       | 0.14          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2 | 35       | 0.14          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2 | 35       | 0.14          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2 | 35       | 0.14          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2 | 39       | 0.14          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2 | 39       | 0.14          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2 | 39       | 0.14          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1 | 6        | 0.14          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2 | 6        | 0.14          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1 | 6        | 0.14          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2 | 6        | 0.14          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1 | 6        | 0.14          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2 | 6        | 0.14          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1 | 11       | 0.14          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2 | 11       | 0.14          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1 | 11       | 0.14          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2 | 11       | 0.14          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1 | 11       | 0.14          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2 | 11       | 0.14          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1 | 27       | 0.14          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2 | 27       | 0.14          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1 | 27       | 0.14          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2 | 27       | 0.14          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1 | 27       | 0.14          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2 | 27       | 0.14          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1 | 34       | 0.14          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2 | 34       | 0.14          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1 | 34       | 0.14          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2 | 34       | 0.14          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1 | 34       | 0.14          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2 | 34       | 0.14          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1 | 38       | 0.14          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2 | 38       | 0.14          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1 | 38       | 0.14          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2 | 38       | 0.14          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1 | 38       | 0.14          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2 | 38       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2073) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 29       | 0.14          |
| (3,2073) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 29       | 0.14          |
| (3,2073) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 29       | 0.14          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD21 | 5        | 0.14          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD22 | 5        | 0.14          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD23 | 5        | 0.14          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD21 | 5        | 0.14          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD22 | 5        | 0.14          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD23 | 5        | 0.14          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD21 | 5        | 0.14          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD22 | 5        | 0.14          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD23 | 5        | 0.14          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD21 | 17       | 0.14          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD22 | 17       | 0.14          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD23 | 17       | 0.14          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD21 | 17       | 0.14          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD22 | 17       | 0.14          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD23 | 17       | 0.14          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD21 | 17       | 0.14          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD22 | 17       | 0.14          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD23 | 17       | 0.14          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1  | 16       | 0.14          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2  | 16       | 0.14          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1  | 16       | 0.14          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2  | 16       | 0.14          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1  | 16       | 0.14          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2  | 16       | 0.14          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1  | 19       | 0.14          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2  | 19       | 0.14          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1  | 19       | 0.14          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2  | 19       | 0.14          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1  | 19       | 0.14          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2  | 19       | 0.14          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 25       | 0.14          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 25       | 0.14          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 25       | 0.14          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 37       | 0.14          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 37       | 0.14          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 37       | 0.14          |
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3  | 2        | 0.14          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3  | 2        | 0.14          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3  | 2        | 0.14          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 8        | 0.14          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 8        | 0.14          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 8        | 0.14          |
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 17       | 0.14          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 17       | 0.14          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 17       | 0.14          |
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 22       | 0.14          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 22       | 0.14          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 22       | 0.14          |
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 28       | 0.14          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 28       | 0.14          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 28       | 0.14          |
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 40       | 0.14          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 40       | 0.14          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 40       | 0.14          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 1        | 0.14          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 1        | 0.14          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 1        | 0.14          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 1        | 0.14          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 1        | 0.14          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 1        | 0.14          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 11       | 0.14          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 11       | 0.14          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 11       | 0.14          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 11       | 0.14          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 11       | 0.14          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 11       | 0.14          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 14       | 0.14          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 14       | 0.14          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 14       | 0.14          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 14       | 0.14          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 14       | 0.14          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 14       | 0.14          |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1 | 17       | 0.14          |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2 | 17       | 0.14          |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3 | 17       | 0.14          |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1 | 17       | 0.14          |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2 | 17       | 0.14          |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3 | 17       | 0.14          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1 | 17       | 0.14          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2 | 17       | 0.14          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3 | 17       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1  | 20       | 0.14          |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2  | 20       | 0.14          |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3  | 20       | 0.14          |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1  | 20       | 0.14          |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2  | 20       | 0.14          |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3  | 20       | 0.14          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1  | 20       | 0.14          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2  | 20       | 0.14          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3  | 20       | 0.14          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 5        | 0.14          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 6        | 0.14          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 7        | 0.14          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 14       | 0.14          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 16       | 0.14          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 27       | 0.14          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 28       | 0.14          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 35       | 0.14          |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 18       | 0.14          |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 18       | 0.14          |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 18       | 0.14          |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 20       | 0.14          |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 20       | 0.14          |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 20       | 0.14          |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 32       | 0.14          |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 32       | 0.14          |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 32       | 0.14          |
| (3,1993) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 9        | 0.14          |
| (3,1993) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 9        | 0.14          |
| (3,1993) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 9        | 0.14          |
| (3,1993) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 28       | 0.14          |
| (3,1993) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 28       | 0.14          |
| (3,1993) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 28       | 0.14          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 14       | 0.14          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 23       | 0.14          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 25       | 0.14          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 28       | 0.14          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 30       | 0.14          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 37       | 0.14          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 39       | 0.14          |
| (3,1959) | 1:72:A:THR:HG21 | 1:74:A:ASP:HB3  | 11       | 0.14          |
| (3,1959) | 1:72:A:THR:HG22 | 1:74:A:ASP:HB3  | 11       | 0.14          |
| (3,1959) | 1:72:A:THR:HG23 | 1:74:A:ASP:HB3  | 11       | 0.14          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1959) | 1:72:A:THR:HG21 | 1:74:A:ASP:HB3 | 36       | 0.14          |
| (3,1959) | 1:72:A:THR:HG22 | 1:74:A:ASP:HB3 | 36       | 0.14          |
| (3,1959) | 1:72:A:THR:HG23 | 1:74:A:ASP:HB3 | 36       | 0.14          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 4        | 0.14          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 4        | 0.14          |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 4        | 0.14          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 14       | 0.14          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 14       | 0.14          |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 14       | 0.14          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 22       | 0.14          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 22       | 0.14          |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 22       | 0.14          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 32       | 0.14          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 32       | 0.14          |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 32       | 0.14          |
| (3,1906) | 1:66:A:MET:HE1  | 1:79:A:TYR:HA  | 7        | 0.14          |
| (3,1906) | 1:66:A:MET:HE2  | 1:79:A:TYR:HA  | 7        | 0.14          |
| (3,1906) | 1:66:A:MET:HE3  | 1:79:A:TYR:HA  | 7        | 0.14          |
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 5        | 0.14          |
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 5        | 0.14          |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 5        | 0.14          |
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 9        | 0.14          |
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 9        | 0.14          |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 9        | 0.14          |
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 13       | 0.14          |
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 13       | 0.14          |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 13       | 0.14          |
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 14       | 0.14          |
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 14       | 0.14          |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 14       | 0.14          |
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 16       | 0.14          |
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 16       | 0.14          |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 16       | 0.14          |
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 23       | 0.14          |
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 23       | 0.14          |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 23       | 0.14          |
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 32       | 0.14          |
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 32       | 0.14          |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 32       | 0.14          |
| (3,1899) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3 | 10       | 0.14          |
| (3,1899) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3 | 10       | 0.14          |
| (3,1899) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3 | 10       | 0.14          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1899) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3 | 37       | 0.14          |
| (3,1899) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3 | 37       | 0.14          |
| (3,1899) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3 | 37       | 0.14          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H   | 6        | 0.14          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H   | 6        | 0.14          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H   | 6        | 0.14          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H   | 17       | 0.14          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H   | 17       | 0.14          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H   | 17       | 0.14          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H   | 20       | 0.14          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H   | 20       | 0.14          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H   | 20       | 0.14          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H   | 25       | 0.14          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H   | 25       | 0.14          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H   | 25       | 0.14          |
| (3,1897) | 1:41:A:THR:HG21 | 1:41:A:THR:H   | 28       | 0.14          |
| (3,1897) | 1:41:A:THR:HG22 | 1:41:A:THR:H   | 28       | 0.14          |
| (3,1897) | 1:41:A:THR:HG23 | 1:41:A:THR:H   | 28       | 0.14          |
| (3,1864) | 1:7:A:ALA:HB1   | 1:88:A:ARG:HA  | 16       | 0.14          |
| (3,1864) | 1:7:A:ALA:HB2   | 1:88:A:ARG:HA  | 16       | 0.14          |
| (3,1864) | 1:7:A:ALA:HB3   | 1:88:A:ARG:HA  | 16       | 0.14          |
| (3,1864) | 1:7:A:ALA:HB1   | 1:88:A:ARG:HA  | 37       | 0.14          |
| (3,1864) | 1:7:A:ALA:HB2   | 1:88:A:ARG:HA  | 37       | 0.14          |
| (3,1864) | 1:7:A:ALA:HB3   | 1:88:A:ARG:HA  | 37       | 0.14          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 17       | 0.14          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 17       | 0.14          |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 17       | 0.14          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 20       | 0.14          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 20       | 0.14          |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 20       | 0.14          |
| (3,1814) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 3        | 0.14          |
| (3,1814) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 4        | 0.14          |
| (3,1814) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 5        | 0.14          |
| (3,1814) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 7        | 0.14          |
| (3,1814) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 10       | 0.14          |
| (3,1814) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 13       | 0.14          |
| (3,1814) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 14       | 0.14          |
| (3,1814) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 15       | 0.14          |
| (3,1814) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 17       | 0.14          |
| (3,1814) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 19       | 0.14          |
| (3,1814) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 20       | 0.14          |
| (3,1814) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 21       | 0.14          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,1814) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 22       | 0.14          |
| (3,1814) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 23       | 0.14          |
| (3,1814) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 24       | 0.14          |
| (3,1814) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 25       | 0.14          |
| (3,1814) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 29       | 0.14          |
| (3,1814) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 30       | 0.14          |
| (3,1814) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 31       | 0.14          |
| (3,1814) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 32       | 0.14          |
| (3,1814) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 34       | 0.14          |
| (3,1814) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 35       | 0.14          |
| (3,1814) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 36       | 0.14          |
| (3,1814) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 38       | 0.14          |
| (3,1814) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 39       | 0.14          |
| (3,1814) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 40       | 0.14          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 15       | 0.14          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 18       | 0.14          |
| (3,1813) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 27       | 0.14          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 15       | 0.14          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG11 | 2        | 0.14          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG12 | 2        | 0.14          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG13 | 2        | 0.14          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG11 | 2        | 0.14          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG12 | 2        | 0.14          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG13 | 2        | 0.14          |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG11 | 2        | 0.14          |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG12 | 2        | 0.14          |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG13 | 2        | 0.14          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG11 | 20       | 0.14          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG12 | 20       | 0.14          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG13 | 20       | 0.14          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG11 | 20       | 0.14          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG12 | 20       | 0.14          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG13 | 20       | 0.14          |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG11 | 20       | 0.14          |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG12 | 20       | 0.14          |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG13 | 20       | 0.14          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG11 | 25       | 0.14          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG12 | 25       | 0.14          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG13 | 25       | 0.14          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG11 | 25       | 0.14          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG12 | 25       | 0.14          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG13 | 25       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 25       | 0.14          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 25       | 0.14          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 25       | 0.14          |
| (3,1712) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 4        | 0.14          |
| (3,1712) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 4        | 0.14          |
| (3,1712) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 4        | 0.14          |
| (3,1712) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 26       | 0.14          |
| (3,1712) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 26       | 0.14          |
| (3,1712) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 26       | 0.14          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 3        | 0.14          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 3        | 0.14          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 3        | 0.14          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 3        | 0.14          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 3        | 0.14          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 3        | 0.14          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 3        | 0.14          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 3        | 0.14          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 3        | 0.14          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 8        | 0.14          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 8        | 0.14          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 8        | 0.14          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 8        | 0.14          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 8        | 0.14          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 8        | 0.14          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 8        | 0.14          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 8        | 0.14          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 8        | 0.14          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 14       | 0.14          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 14       | 0.14          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 14       | 0.14          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 14       | 0.14          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 14       | 0.14          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 14       | 0.14          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 14       | 0.14          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 14       | 0.14          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 14       | 0.14          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 26       | 0.14          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 26       | 0.14          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 26       | 0.14          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 26       | 0.14          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 26       | 0.14          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 26       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 26       | 0.14          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 26       | 0.14          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 26       | 0.14          |
| (3,1683) | 1:85:A:LEU:HD11 | 1:35:A:PHE:HD1  | 5        | 0.14          |
| (3,1683) | 1:85:A:LEU:HD11 | 1:35:A:PHE:HD2  | 5        | 0.14          |
| (3,1683) | 1:85:A:LEU:HD12 | 1:35:A:PHE:HD1  | 5        | 0.14          |
| (3,1683) | 1:85:A:LEU:HD12 | 1:35:A:PHE:HD2  | 5        | 0.14          |
| (3,1683) | 1:85:A:LEU:HD13 | 1:35:A:PHE:HD1  | 5        | 0.14          |
| (3,1683) | 1:85:A:LEU:HD13 | 1:35:A:PHE:HD2  | 5        | 0.14          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 32       | 0.14          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 32       | 0.14          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 32       | 0.14          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 32       | 0.14          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 32       | 0.14          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 32       | 0.14          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 32       | 0.14          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 32       | 0.14          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 32       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 1        | 0.14          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 1        | 0.14          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 1        | 0.14          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 5        | 0.14          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 5        | 0.14          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 5        | 0.14          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 8        | 0.14          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 8        | 0.14          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 8        | 0.14          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 11       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 11       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 11       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 13       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 13       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 13       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 21       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 21       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 21       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 22       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 22       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 22       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 24       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 24       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 24       | 0.14          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H   | 27       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H   | 27       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 27       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H   | 30       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H   | 30       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 30       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H   | 31       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H   | 31       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 31       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H   | 32       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H   | 32       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 32       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H   | 34       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H   | 34       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 34       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H   | 38       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H   | 38       | 0.14          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 38       | 0.14          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2 | 1        | 0.14          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 1        | 0.14          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 1        | 0.14          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2 | 14       | 0.14          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 14       | 0.14          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 14       | 0.14          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2 | 22       | 0.14          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 22       | 0.14          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 22       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 3        | 0.14          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 3        | 0.14          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 3        | 0.14          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 3        | 0.14          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 3        | 0.14          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 3        | 0.14          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 11       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 11       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 11       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 11       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 11       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 11       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 14       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 14       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 14       | 0.14          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 14       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 14       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 14       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 15       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 15       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 15       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 15       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 15       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 15       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 21       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 21       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 21       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 21       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 21       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 21       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 22       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 22       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 22       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 22       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 22       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 22       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 23       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 23       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 23       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 23       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 23       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 23       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 25       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 25       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 25       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 25       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 25       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 25       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 27       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 27       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 27       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 27       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 27       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 27       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 30       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 30       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 30       | 0.14          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 30       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 30       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 30       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 38       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 38       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 38       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 38       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 38       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 38       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 39       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 39       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 39       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 39       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 39       | 0.14          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 39       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 2        | 0.14          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 2        | 0.14          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 2        | 0.14          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 2        | 0.14          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 2        | 0.14          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 2        | 0.14          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 22       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 22       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 22       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 22       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 22       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 22       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 24       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 24       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 24       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 24       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 24       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 24       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 25       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 25       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 25       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 25       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 25       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 25       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 34       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 34       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 34       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 34       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 34       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 34       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 35       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 35       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 35       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 35       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 35       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 35       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 36       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 36       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 36       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 36       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 36       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 36       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 38       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 38       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 38       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 38       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 38       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 38       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 39       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 39       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 39       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 39       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 39       | 0.14          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 39       | 0.14          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 9        | 0.14          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 9        | 0.14          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 9        | 0.14          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 10       | 0.14          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 10       | 0.14          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 10       | 0.14          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 16       | 0.14          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 16       | 0.14          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 16       | 0.14          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 17       | 0.14          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 17       | 0.14          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 17       | 0.14          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 19       | 0.14          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 19       | 0.14          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 19       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 28       | 0.14          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 28       | 0.14          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 28       | 0.14          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 3        | 0.14          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 3        | 0.14          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 3        | 0.14          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 7        | 0.14          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 7        | 0.14          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 7        | 0.14          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 8        | 0.14          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 8        | 0.14          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 8        | 0.14          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 12       | 0.14          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 12       | 0.14          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 12       | 0.14          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 16       | 0.14          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 16       | 0.14          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 16       | 0.14          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 29       | 0.14          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 29       | 0.14          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 29       | 0.14          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 33       | 0.14          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 33       | 0.14          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 33       | 0.14          |
| (3,1563) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 36       | 0.14          |
| (3,1563) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 36       | 0.14          |
| (3,1563) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 36       | 0.14          |
| (3,1554) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA    | 29       | 0.14          |
| (3,1554) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA    | 29       | 0.14          |
| (3,1554) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA    | 29       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H    | 3        | 0.14          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H    | 3        | 0.14          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H    | 3        | 0.14          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H    | 5        | 0.14          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H    | 5        | 0.14          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H    | 5        | 0.14          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H    | 6        | 0.14          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H    | 6        | 0.14          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H    | 6        | 0.14          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H    | 7        | 0.14          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H    | 7        | 0.14          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H    | 7        | 0.14          |

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| Key      | Atom-1          | Atom-2       | Model ID | Violation (Å) |
|----------|-----------------|--------------|----------|---------------|
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 9        | 0.14          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 9        | 0.14          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 9        | 0.14          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 10       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 10       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 10       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 12       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 12       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 12       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 16       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 16       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 16       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 17       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 17       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 17       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 18       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 18       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 18       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 19       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 19       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 19       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 20       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 20       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 20       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 23       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 23       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 23       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 25       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 25       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 25       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 26       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 26       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 26       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 29       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 29       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 29       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 30       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 30       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 30       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 31       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 31       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 31       | 0.14          |

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| Key      | Atom-1          | Atom-2       | Model ID | Violation (Å) |
|----------|-----------------|--------------|----------|---------------|
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 32       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 32       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 32       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 33       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 33       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 33       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 34       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 34       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 34       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 37       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 37       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 37       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 38       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 38       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 38       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 39       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 39       | 0.14          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 39       | 0.14          |
| (3,1539) | 1:2:A:ILE:HD11  | 1:2:A:ILE:HA | 29       | 0.14          |
| (3,1539) | 1:2:A:ILE:HD12  | 1:2:A:ILE:HA | 29       | 0.14          |
| (3,1539) | 1:2:A:ILE:HD13  | 1:2:A:ILE:HA | 29       | 0.14          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H | 2        | 0.14          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H | 2        | 0.14          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H | 2        | 0.14          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H | 7        | 0.14          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H | 7        | 0.14          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H | 7        | 0.14          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H | 11       | 0.14          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H | 11       | 0.14          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H | 11       | 0.14          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H | 18       | 0.14          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H | 18       | 0.14          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H | 18       | 0.14          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H | 23       | 0.14          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H | 23       | 0.14          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H | 23       | 0.14          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H | 25       | 0.14          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H | 25       | 0.14          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H | 25       | 0.14          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H | 30       | 0.14          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H | 30       | 0.14          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H | 30       | 0.14          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,1518) | 1:66:A:MET:HE1 | 1:66:A:MET:H   | 31       | 0.14          |
| (3,1518) | 1:66:A:MET:HE2 | 1:66:A:MET:H   | 31       | 0.14          |
| (3,1518) | 1:66:A:MET:HE3 | 1:66:A:MET:H   | 31       | 0.14          |
| (3,1518) | 1:66:A:MET:HE1 | 1:66:A:MET:H   | 33       | 0.14          |
| (3,1518) | 1:66:A:MET:HE2 | 1:66:A:MET:H   | 33       | 0.14          |
| (3,1518) | 1:66:A:MET:HE3 | 1:66:A:MET:H   | 33       | 0.14          |
| (3,1518) | 1:66:A:MET:HE1 | 1:66:A:MET:H   | 39       | 0.14          |
| (3,1518) | 1:66:A:MET:HE2 | 1:66:A:MET:H   | 39       | 0.14          |
| (3,1518) | 1:66:A:MET:HE3 | 1:66:A:MET:H   | 39       | 0.14          |
| (3,1517) | 1:66:A:MET:HE1 | 1:29:A:PHE:H   | 1        | 0.14          |
| (3,1517) | 1:66:A:MET:HE2 | 1:29:A:PHE:H   | 1        | 0.14          |
| (3,1517) | 1:66:A:MET:HE3 | 1:29:A:PHE:H   | 1        | 0.14          |
| (3,1517) | 1:66:A:MET:HE1 | 1:29:A:PHE:H   | 5        | 0.14          |
| (3,1517) | 1:66:A:MET:HE2 | 1:29:A:PHE:H   | 5        | 0.14          |
| (3,1517) | 1:66:A:MET:HE3 | 1:29:A:PHE:H   | 5        | 0.14          |
| (3,1517) | 1:66:A:MET:HE1 | 1:29:A:PHE:H   | 23       | 0.14          |
| (3,1517) | 1:66:A:MET:HE2 | 1:29:A:PHE:H   | 23       | 0.14          |
| (3,1517) | 1:66:A:MET:HE3 | 1:29:A:PHE:H   | 23       | 0.14          |
| (3,1517) | 1:66:A:MET:HE1 | 1:29:A:PHE:H   | 37       | 0.14          |
| (3,1517) | 1:66:A:MET:HE2 | 1:29:A:PHE:H   | 37       | 0.14          |
| (3,1517) | 1:66:A:MET:HE3 | 1:29:A:PHE:H   | 37       | 0.14          |
| (3,1514) | 1:66:A:MET:HE1 | 1:42:A:TRP:HE1 | 16       | 0.14          |
| (3,1514) | 1:66:A:MET:HE2 | 1:42:A:TRP:HE1 | 16       | 0.14          |
| (3,1514) | 1:66:A:MET:HE3 | 1:42:A:TRP:HE1 | 16       | 0.14          |
| (3,1514) | 1:66:A:MET:HE1 | 1:42:A:TRP:HE1 | 28       | 0.14          |
| (3,1514) | 1:66:A:MET:HE2 | 1:42:A:TRP:HE1 | 28       | 0.14          |
| (3,1514) | 1:66:A:MET:HE3 | 1:42:A:TRP:HE1 | 28       | 0.14          |
| (3,1514) | 1:66:A:MET:HE1 | 1:42:A:TRP:HE1 | 33       | 0.14          |
| (3,1514) | 1:66:A:MET:HE2 | 1:42:A:TRP:HE1 | 33       | 0.14          |
| (3,1514) | 1:66:A:MET:HE3 | 1:42:A:TRP:HE1 | 33       | 0.14          |
| (3,1514) | 1:66:A:MET:HE1 | 1:42:A:TRP:HE1 | 39       | 0.14          |
| (3,1514) | 1:66:A:MET:HE2 | 1:42:A:TRP:HE1 | 39       | 0.14          |
| (3,1514) | 1:66:A:MET:HE3 | 1:42:A:TRP:HE1 | 39       | 0.14          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 4        | 0.14          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 4        | 0.14          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 4        | 0.14          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 4        | 0.14          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 4        | 0.14          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 4        | 0.14          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 7        | 0.14          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 7        | 0.14          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 7        | 0.14          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 7        | 0.14          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 7        | 0.14          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 7        | 0.14          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 12       | 0.14          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 12       | 0.14          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 12       | 0.14          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 12       | 0.14          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 12       | 0.14          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 12       | 0.14          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 21       | 0.14          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 21       | 0.14          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 21       | 0.14          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 21       | 0.14          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 21       | 0.14          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 21       | 0.14          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 23       | 0.14          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 23       | 0.14          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 23       | 0.14          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 23       | 0.14          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 23       | 0.14          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 23       | 0.14          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 40       | 0.14          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 40       | 0.14          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 40       | 0.14          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 40       | 0.14          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 40       | 0.14          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 40       | 0.14          |
| (3,1512) | 1:66:A:MET:HE1 | 1:42:A:TRP:HZ3 | 8        | 0.14          |
| (3,1512) | 1:66:A:MET:HE2 | 1:42:A:TRP:HZ3 | 8        | 0.14          |
| (3,1512) | 1:66:A:MET:HE3 | 1:42:A:TRP:HZ3 | 8        | 0.14          |
| (3,1512) | 1:66:A:MET:HE1 | 1:42:A:TRP:HZ3 | 13       | 0.14          |
| (3,1512) | 1:66:A:MET:HE2 | 1:42:A:TRP:HZ3 | 13       | 0.14          |
| (3,1512) | 1:66:A:MET:HE3 | 1:42:A:TRP:HZ3 | 13       | 0.14          |
| (3,1512) | 1:66:A:MET:HE1 | 1:42:A:TRP:HZ3 | 18       | 0.14          |
| (3,1512) | 1:66:A:MET:HE2 | 1:42:A:TRP:HZ3 | 18       | 0.14          |
| (3,1512) | 1:66:A:MET:HE3 | 1:42:A:TRP:HZ3 | 18       | 0.14          |
| (3,1512) | 1:66:A:MET:HE1 | 1:42:A:TRP:HZ3 | 35       | 0.14          |
| (3,1512) | 1:66:A:MET:HE2 | 1:42:A:TRP:HZ3 | 35       | 0.14          |
| (3,1512) | 1:66:A:MET:HE3 | 1:42:A:TRP:HZ3 | 35       | 0.14          |
| (3,1511) | 1:66:A:MET:HE1 | 1:42:A:TRP:HB2 | 27       | 0.14          |
| (3,1511) | 1:66:A:MET:HE2 | 1:42:A:TRP:HB2 | 27       | 0.14          |
| (3,1511) | 1:66:A:MET:HE3 | 1:42:A:TRP:HB2 | 27       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1506) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD11 | 27       | 0.14          |
| (3,1506) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD12 | 27       | 0.14          |
| (3,1506) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD13 | 27       | 0.14          |
| (3,1506) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD11 | 27       | 0.14          |
| (3,1506) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD12 | 27       | 0.14          |
| (3,1506) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD13 | 27       | 0.14          |
| (3,1506) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD11 | 27       | 0.14          |
| (3,1506) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD12 | 27       | 0.14          |
| (3,1506) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD13 | 27       | 0.14          |
| (3,1504) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2  | 4        | 0.14          |
| (3,1504) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2  | 4        | 0.14          |
| (3,1504) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2  | 4        | 0.14          |
| (3,1504) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2  | 15       | 0.14          |
| (3,1504) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2  | 15       | 0.14          |
| (3,1504) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2  | 15       | 0.14          |
| (3,1504) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2  | 16       | 0.14          |
| (3,1504) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2  | 16       | 0.14          |
| (3,1504) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2  | 16       | 0.14          |
| (3,1504) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2  | 29       | 0.14          |
| (3,1504) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2  | 29       | 0.14          |
| (3,1504) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2  | 29       | 0.14          |
| (3,1504) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2  | 39       | 0.14          |
| (3,1504) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2  | 39       | 0.14          |
| (3,1504) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2  | 39       | 0.14          |
| (3,1498) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 9        | 0.14          |
| (3,1498) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 9        | 0.14          |
| (3,1498) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 9        | 0.14          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA   | 7        | 0.14          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA   | 7        | 0.14          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA   | 7        | 0.14          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA   | 31       | 0.14          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA   | 31       | 0.14          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA   | 31       | 0.14          |
| (3,1488) | 1:81:A:VAL:HB   | 1:42:A:TRP:HE1  | 5        | 0.14          |
| (3,1488) | 1:81:A:VAL:HB   | 1:42:A:TRP:HE1  | 14       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H    | 1        | 0.14          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H    | 1        | 0.14          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H    | 1        | 0.14          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H    | 2        | 0.14          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H    | 2        | 0.14          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H    | 2        | 0.14          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H    | 4        | 0.14          |

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| Key      | Atom-1          | Atom-2       | Model ID | Violation (Å) |
|----------|-----------------|--------------|----------|---------------|
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 4        | 0.14          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 4        | 0.14          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 9        | 0.14          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 9        | 0.14          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 9        | 0.14          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 10       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 10       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 10       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 15       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 15       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 15       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 18       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 18       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 18       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 22       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 22       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 22       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 26       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 26       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 26       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 27       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 27       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 27       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 31       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 31       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 31       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 32       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 32       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 32       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 35       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 35       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 35       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 39       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 39       | 0.14          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 39       | 0.14          |
| (3,1467) | 1:71:A:VAL:HG21 | 1:72:A:THR:H | 18       | 0.14          |
| (3,1467) | 1:71:A:VAL:HG22 | 1:72:A:THR:H | 18       | 0.14          |
| (3,1467) | 1:71:A:VAL:HG23 | 1:72:A:THR:H | 18       | 0.14          |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H | 1        | 0.14          |
| (3,1407) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H | 1        | 0.14          |
| (3,1407) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H | 1        | 0.14          |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H | 4        | 0.14          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,1407) | 1:95:A:ALA:HB2 | 1:18:A:ASN:H    | 4        | 0.14          |
| (3,1407) | 1:95:A:ALA:HB3 | 1:18:A:ASN:H    | 4        | 0.14          |
| (3,1407) | 1:95:A:ALA:HB1 | 1:18:A:ASN:H    | 10       | 0.14          |
| (3,1407) | 1:95:A:ALA:HB2 | 1:18:A:ASN:H    | 10       | 0.14          |
| (3,1407) | 1:95:A:ALA:HB3 | 1:18:A:ASN:H    | 10       | 0.14          |
| (3,1407) | 1:95:A:ALA:HB1 | 1:18:A:ASN:H    | 16       | 0.14          |
| (3,1407) | 1:95:A:ALA:HB2 | 1:18:A:ASN:H    | 16       | 0.14          |
| (3,1407) | 1:95:A:ALA:HB3 | 1:18:A:ASN:H    | 16       | 0.14          |
| (3,1407) | 1:95:A:ALA:HB1 | 1:18:A:ASN:H    | 27       | 0.14          |
| (3,1407) | 1:95:A:ALA:HB2 | 1:18:A:ASN:H    | 27       | 0.14          |
| (3,1407) | 1:95:A:ALA:HB3 | 1:18:A:ASN:H    | 27       | 0.14          |
| (3,1407) | 1:95:A:ALA:HB1 | 1:18:A:ASN:H    | 29       | 0.14          |
| (3,1407) | 1:95:A:ALA:HB2 | 1:18:A:ASN:H    | 29       | 0.14          |
| (3,1407) | 1:95:A:ALA:HB3 | 1:18:A:ASN:H    | 29       | 0.14          |
| (3,1407) | 1:95:A:ALA:HB1 | 1:18:A:ASN:H    | 34       | 0.14          |
| (3,1407) | 1:95:A:ALA:HB2 | 1:18:A:ASN:H    | 34       | 0.14          |
| (3,1407) | 1:95:A:ALA:HB3 | 1:18:A:ASN:H    | 34       | 0.14          |
| (3,1407) | 1:95:A:ALA:HB1 | 1:18:A:ASN:H    | 39       | 0.14          |
| (3,1407) | 1:95:A:ALA:HB2 | 1:18:A:ASN:H    | 39       | 0.14          |
| (3,1407) | 1:95:A:ALA:HB3 | 1:18:A:ASN:H    | 39       | 0.14          |
| (3,1405) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H    | 9        | 0.14          |
| (3,1405) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H    | 9        | 0.14          |
| (3,1405) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 9        | 0.14          |
| (3,1405) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H    | 36       | 0.14          |
| (3,1405) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H    | 36       | 0.14          |
| (3,1405) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 36       | 0.14          |
| (3,1405) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H    | 38       | 0.14          |
| (3,1405) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H    | 38       | 0.14          |
| (3,1405) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 38       | 0.14          |
| (3,1405) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H    | 39       | 0.14          |
| (3,1405) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H    | 39       | 0.14          |
| (3,1405) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 39       | 0.14          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 2        | 0.14          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 2        | 0.14          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 2        | 0.14          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 3        | 0.14          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 3        | 0.14          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 3        | 0.14          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 4        | 0.14          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 4        | 0.14          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 4        | 0.14          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 5        | 0.14          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 5        | 0.14          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 5        | 0.14          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 6        | 0.14          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 6        | 0.14          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 6        | 0.14          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 14       | 0.14          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 14       | 0.14          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 14       | 0.14          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 16       | 0.14          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 16       | 0.14          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 16       | 0.14          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 22       | 0.14          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 22       | 0.14          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 22       | 0.14          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 25       | 0.14          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 25       | 0.14          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 25       | 0.14          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 27       | 0.14          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 27       | 0.14          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 27       | 0.14          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 31       | 0.14          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 31       | 0.14          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 31       | 0.14          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 32       | 0.14          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 32       | 0.14          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 32       | 0.14          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 39       | 0.14          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 39       | 0.14          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 39       | 0.14          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 40       | 0.14          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 40       | 0.14          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 40       | 0.14          |
| (3,1391) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ   | 3        | 0.14          |
| (3,1391) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ   | 3        | 0.14          |
| (3,1391) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ   | 3        | 0.14          |
| (3,1391) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ   | 5        | 0.14          |
| (3,1391) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ   | 5        | 0.14          |
| (3,1391) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ   | 5        | 0.14          |
| (3,1391) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ   | 10       | 0.14          |
| (3,1391) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ   | 10       | 0.14          |
| (3,1391) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ   | 10       | 0.14          |
| (3,1391) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ   | 35       | 0.14          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,1391) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ  | 35       | 0.14          |
| (3,1391) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ  | 35       | 0.14          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 24       | 0.14          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 24       | 0.14          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 24       | 0.14          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 24       | 0.14          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 24       | 0.14          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 24       | 0.14          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 24       | 0.14          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 24       | 0.14          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 24       | 0.14          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 40       | 0.14          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 40       | 0.14          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 40       | 0.14          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 40       | 0.14          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 40       | 0.14          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 40       | 0.14          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 40       | 0.14          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 40       | 0.14          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 40       | 0.14          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 24       | 0.14          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 24       | 0.14          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 24       | 0.14          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 24       | 0.14          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 24       | 0.14          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 24       | 0.14          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 24       | 0.14          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 24       | 0.14          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 24       | 0.14          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 40       | 0.14          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 40       | 0.14          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 40       | 0.14          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 40       | 0.14          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 40       | 0.14          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 40       | 0.14          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 40       | 0.14          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 40       | 0.14          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 40       | 0.14          |
| (3,1372) | 1:16:A:ILE:HB  | 1:29:A:PHE:HB3 | 6        | 0.14          |
| (3,1372) | 1:16:A:ILE:HB  | 1:29:A:PHE:HB3 | 16       | 0.14          |
| (3,1372) | 1:16:A:ILE:HB  | 1:29:A:PHE:HB3 | 33       | 0.14          |
| (3,1329) | 1:19:A:ILE:HB  | 1:20:A:VAL:H   | 4        | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 10       | 0.14          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 11       | 0.14          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 14       | 0.14          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 15       | 0.14          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 19       | 0.14          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 20       | 0.14          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 23       | 0.14          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 25       | 0.14          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 26       | 0.14          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 29       | 0.14          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 30       | 0.14          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 31       | 0.14          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 32       | 0.14          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 33       | 0.14          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 35       | 0.14          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 36       | 0.14          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 37       | 0.14          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 39       | 0.14          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 40       | 0.14          |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 9        | 0.14          |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 15       | 0.14          |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 29       | 0.14          |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 35       | 0.14          |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 36       | 0.14          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 12       | 0.14          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 12       | 0.14          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 12       | 0.14          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 19       | 0.14          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 19       | 0.14          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 19       | 0.14          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 21       | 0.14          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 21       | 0.14          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 21       | 0.14          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 31       | 0.14          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 31       | 0.14          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 31       | 0.14          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1  | 17       | 0.14          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2  | 17       | 0.14          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3  | 17       | 0.14          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1  | 17       | 0.14          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2  | 17       | 0.14          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3  | 17       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1  | 17       | 0.14          |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2  | 17       | 0.14          |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3  | 17       | 0.14          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1  | 20       | 0.14          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2  | 20       | 0.14          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3  | 20       | 0.14          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1  | 20       | 0.14          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2  | 20       | 0.14          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3  | 20       | 0.14          |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1  | 20       | 0.14          |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2  | 20       | 0.14          |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3  | 20       | 0.14          |
| (3,1293) | 1:40:A:VAL:HG21 | 1:42:A:TRP:HE1  | 35       | 0.14          |
| (3,1293) | 1:40:A:VAL:HG22 | 1:42:A:TRP:HE1  | 35       | 0.14          |
| (3,1293) | 1:40:A:VAL:HG23 | 1:42:A:TRP:HE1  | 35       | 0.14          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 12       | 0.14          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 12       | 0.14          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 12       | 0.14          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 19       | 0.14          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 19       | 0.14          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 19       | 0.14          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 21       | 0.14          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 21       | 0.14          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 21       | 0.14          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 31       | 0.14          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 31       | 0.14          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 31       | 0.14          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 1        | 0.14          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 1        | 0.14          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 1        | 0.14          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 1        | 0.14          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 1        | 0.14          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 1        | 0.14          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 1        | 0.14          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 1        | 0.14          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 1        | 0.14          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 4        | 0.14          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 4        | 0.14          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 4        | 0.14          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 4        | 0.14          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 4        | 0.14          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 4        | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 4        | 0.14          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 4        | 0.14          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 4        | 0.14          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 17       | 0.14          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 17       | 0.14          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 17       | 0.14          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 17       | 0.14          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 17       | 0.14          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 17       | 0.14          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 17       | 0.14          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 17       | 0.14          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 17       | 0.14          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 18       | 0.14          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 18       | 0.14          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 18       | 0.14          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 18       | 0.14          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 18       | 0.14          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 18       | 0.14          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 18       | 0.14          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 18       | 0.14          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 18       | 0.14          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 22       | 0.14          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 22       | 0.14          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 22       | 0.14          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 22       | 0.14          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 22       | 0.14          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 22       | 0.14          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 22       | 0.14          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 22       | 0.14          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 22       | 0.14          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 30       | 0.14          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 30       | 0.14          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 30       | 0.14          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 30       | 0.14          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 30       | 0.14          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 30       | 0.14          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 30       | 0.14          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 30       | 0.14          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 30       | 0.14          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 34       | 0.14          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 34       | 0.14          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 34       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 34       | 0.14          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 34       | 0.14          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 34       | 0.14          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 34       | 0.14          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 34       | 0.14          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 34       | 0.14          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 10       | 0.14          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 10       | 0.14          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 10       | 0.14          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 11       | 0.14          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 11       | 0.14          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 11       | 0.14          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 13       | 0.14          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 13       | 0.14          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 13       | 0.14          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 33       | 0.14          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 33       | 0.14          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 33       | 0.14          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 34       | 0.14          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 34       | 0.14          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 34       | 0.14          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 35       | 0.14          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 35       | 0.14          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 35       | 0.14          |
| (3,1267) | 1:94:A:THR:HG21 | 1:94:A:THR:HA   | 28       | 0.14          |
| (3,1267) | 1:94:A:THR:HG22 | 1:94:A:THR:HA   | 28       | 0.14          |
| (3,1267) | 1:94:A:THR:HG23 | 1:94:A:THR:HA   | 28       | 0.14          |
| (3,1265) | 1:67:A:THR:HG21 | 1:56:A:ASN:H    | 23       | 0.14          |
| (3,1265) | 1:67:A:THR:HG22 | 1:56:A:ASN:H    | 23       | 0.14          |
| (3,1265) | 1:67:A:THR:HG23 | 1:56:A:ASN:H    | 23       | 0.14          |
| (3,1261) | 1:67:A:THR:HG21 | 1:26:A:SER:HB2  | 4        | 0.14          |
| (3,1261) | 1:67:A:THR:HG22 | 1:26:A:SER:HB2  | 4        | 0.14          |
| (3,1261) | 1:67:A:THR:HG23 | 1:26:A:SER:HB2  | 4        | 0.14          |
| (3,1261) | 1:67:A:THR:HG21 | 1:26:A:SER:HB2  | 30       | 0.14          |
| (3,1261) | 1:67:A:THR:HG22 | 1:26:A:SER:HB2  | 30       | 0.14          |
| (3,1261) | 1:67:A:THR:HG23 | 1:26:A:SER:HB2  | 30       | 0.14          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 22       | 0.14          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 22       | 0.14          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 22       | 0.14          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 30       | 0.14          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 30       | 0.14          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 30       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 31       | 0.14          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 31       | 0.14          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 31       | 0.14          |
| (3,1252) | 1:28:A:THR:HG21 | 1:67:A:THR:HG21 | 9        | 0.14          |
| (3,1252) | 1:28:A:THR:HG21 | 1:67:A:THR:HG22 | 9        | 0.14          |
| (3,1252) | 1:28:A:THR:HG21 | 1:67:A:THR:HG23 | 9        | 0.14          |
| (3,1252) | 1:28:A:THR:HG22 | 1:67:A:THR:HG21 | 9        | 0.14          |
| (3,1252) | 1:28:A:THR:HG22 | 1:67:A:THR:HG22 | 9        | 0.14          |
| (3,1252) | 1:28:A:THR:HG22 | 1:67:A:THR:HG23 | 9        | 0.14          |
| (3,1252) | 1:28:A:THR:HG23 | 1:67:A:THR:HG21 | 9        | 0.14          |
| (3,1252) | 1:28:A:THR:HG23 | 1:67:A:THR:HG22 | 9        | 0.14          |
| (3,1252) | 1:28:A:THR:HG23 | 1:67:A:THR:HG23 | 9        | 0.14          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 1        | 0.14          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 1        | 0.14          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 1        | 0.14          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 7        | 0.14          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 7        | 0.14          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 7        | 0.14          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 17       | 0.14          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 17       | 0.14          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 17       | 0.14          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 19       | 0.14          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 19       | 0.14          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 19       | 0.14          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 24       | 0.14          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 24       | 0.14          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 24       | 0.14          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 25       | 0.14          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 25       | 0.14          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 25       | 0.14          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 34       | 0.14          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 34       | 0.14          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 34       | 0.14          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 35       | 0.14          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 35       | 0.14          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 35       | 0.14          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 39       | 0.14          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 39       | 0.14          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 39       | 0.14          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 40       | 0.14          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 40       | 0.14          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 40       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1243) | 1:13:A:THR:HG21 | 1:34:A:SER:H    | 21       | 0.14          |
| (3,1243) | 1:13:A:THR:HG22 | 1:34:A:SER:H    | 21       | 0.14          |
| (3,1243) | 1:13:A:THR:HG23 | 1:34:A:SER:H    | 21       | 0.14          |
| (3,1243) | 1:13:A:THR:HG21 | 1:34:A:SER:H    | 32       | 0.14          |
| (3,1243) | 1:13:A:THR:HG22 | 1:34:A:SER:H    | 32       | 0.14          |
| (3,1243) | 1:13:A:THR:HG23 | 1:34:A:SER:H    | 32       | 0.14          |
| (3,1240) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3  | 15       | 0.14          |
| (3,1240) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3  | 15       | 0.14          |
| (3,1240) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3  | 15       | 0.14          |
| (3,1240) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3  | 25       | 0.14          |
| (3,1240) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3  | 25       | 0.14          |
| (3,1240) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3  | 25       | 0.14          |
| (3,1230) | 1:101:A:LEU:H   | 1:22:A:SER:HA   | 6        | 0.14          |
| (3,1230) | 1:101:A:LEU:H   | 1:22:A:SER:HA   | 7        | 0.14          |
| (3,1230) | 1:101:A:LEU:H   | 1:22:A:SER:HA   | 19       | 0.14          |
| (3,1230) | 1:101:A:LEU:H   | 1:22:A:SER:HA   | 26       | 0.14          |
| (3,1230) | 1:101:A:LEU:H   | 1:22:A:SER:HA   | 39       | 0.14          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 20       | 0.14          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 20       | 0.14          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 20       | 0.14          |
| (3,1217) | 1:66:A:MET:H    | 1:28:A:THR:HA   | 4        | 0.14          |
| (3,1217) | 1:66:A:MET:H    | 1:28:A:THR:HA   | 7        | 0.14          |
| (3,1217) | 1:66:A:MET:H    | 1:28:A:THR:HA   | 31       | 0.14          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 24       | 0.14          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 24       | 0.14          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 24       | 0.14          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 33       | 0.14          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 33       | 0.14          |
| (3,1194) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 33       | 0.14          |
| (3,1189) | 1:21:A:VAL:H    | 1:100:A:GLU:HB3 | 14       | 0.14          |
| (3,1181) | 1:100:A:GLU:H   | 1:21:A:VAL:HG11 | 15       | 0.14          |
| (3,1181) | 1:100:A:GLU:H   | 1:21:A:VAL:HG12 | 15       | 0.14          |
| (3,1181) | 1:100:A:GLU:H   | 1:21:A:VAL:HG13 | 15       | 0.14          |
| (3,1178) | 1:91:A:ALA:H    | 1:84:A:ARG:HA   | 11       | 0.14          |
| (3,1178) | 1:91:A:ALA:H    | 1:84:A:ARG:HA   | 15       | 0.14          |
| (3,1166) | 1:97:A:LEU:H    | 1:29:A:PHE:HE1  | 23       | 0.14          |
| (3,1166) | 1:97:A:LEU:H    | 1:29:A:PHE:HE2  | 23       | 0.14          |
| (3,1166) | 1:97:A:LEU:H    | 1:29:A:PHE:HE1  | 30       | 0.14          |
| (3,1166) | 1:97:A:LEU:H    | 1:29:A:PHE:HE2  | 30       | 0.14          |
| (3,1166) | 1:97:A:LEU:H    | 1:29:A:PHE:HE1  | 36       | 0.14          |
| (3,1166) | 1:97:A:LEU:H    | 1:29:A:PHE:HE2  | 36       | 0.14          |
| (3,1096) | 1:74:A:ASP:H    | 1:73:A:PRO:HA   | 30       | 0.14          |

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| Key      | Atom-1       | Atom-2         | Model ID | Violation (Å) |
|----------|--------------|----------------|----------|---------------|
| (3,1096) | 1:74:A:ASP:H | 1:73:A:PRO:HA  | 32       | 0.14          |
| (3,1096) | 1:74:A:ASP:H | 1:73:A:PRO:HA  | 35       | 0.14          |
| (3,1096) | 1:74:A:ASP:H | 1:73:A:PRO:HA  | 37       | 0.14          |
| (3,1096) | 1:74:A:ASP:H | 1:73:A:PRO:HA  | 38       | 0.14          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 6        | 0.14          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 7        | 0.14          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 9        | 0.14          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 15       | 0.14          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 25       | 0.14          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 27       | 0.14          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 28       | 0.14          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 30       | 0.14          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 32       | 0.14          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 34       | 0.14          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 35       | 0.14          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 36       | 0.14          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 37       | 0.14          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 38       | 0.14          |
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 10       | 0.14          |
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 16       | 0.14          |
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 18       | 0.14          |
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 26       | 0.14          |
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 28       | 0.14          |
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 31       | 0.14          |
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 34       | 0.14          |
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 35       | 0.14          |
| (3,1042) | 1:26:A:SER:H | 1:26:A:SER:HB3 | 14       | 0.14          |
| (3,1042) | 1:26:A:SER:H | 1:26:A:SER:HB3 | 26       | 0.14          |
| (3,1019) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 9        | 0.14          |
| (3,1019) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 17       | 0.14          |
| (3,1019) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 18       | 0.14          |
| (3,1019) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 35       | 0.14          |
| (3,1003) | 1:5:A:PHE:H  | 1:4:A:PRO:HA   | 29       | 0.14          |
| (3,988)  | 1:12:A:PHE:H | 1:11:A:GLN:HB2 | 5        | 0.14          |
| (3,988)  | 1:12:A:PHE:H | 1:11:A:GLN:HB2 | 21       | 0.14          |
| (3,988)  | 1:12:A:PHE:H | 1:11:A:GLN:HB2 | 23       | 0.14          |
| (3,988)  | 1:12:A:PHE:H | 1:11:A:GLN:HB2 | 27       | 0.14          |
| (3,988)  | 1:12:A:PHE:H | 1:11:A:GLN:HB2 | 31       | 0.14          |
| (3,988)  | 1:12:A:PHE:H | 1:11:A:GLN:HB2 | 39       | 0.14          |
| (3,979)  | 1:20:A:VAL:H | 1:19:A:ILE:HB  | 4        | 0.14          |
| (3,979)  | 1:20:A:VAL:H | 1:19:A:ILE:HB  | 10       | 0.14          |
| (3,979)  | 1:20:A:VAL:H | 1:19:A:ILE:HB  | 11       | 0.14          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 14       | 0.14          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 15       | 0.14          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 19       | 0.14          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 20       | 0.14          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 23       | 0.14          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 25       | 0.14          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 26       | 0.14          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 29       | 0.14          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 30       | 0.14          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 31       | 0.14          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 32       | 0.14          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 33       | 0.14          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 35       | 0.14          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 36       | 0.14          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 37       | 0.14          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 39       | 0.14          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 40       | 0.14          |
| (3,972) | 1:21:A:VAL:H | 1:21:A:VAL:HG21 | 6        | 0.14          |
| (3,972) | 1:21:A:VAL:H | 1:21:A:VAL:HG22 | 6        | 0.14          |
| (3,972) | 1:21:A:VAL:H | 1:21:A:VAL:HG23 | 6        | 0.14          |
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 1        | 0.14          |
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 13       | 0.14          |
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 23       | 0.14          |
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 26       | 0.14          |
| (3,942) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 8        | 0.14          |
| (3,942) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 16       | 0.14          |
| (3,942) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 21       | 0.14          |
| (3,942) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 22       | 0.14          |
| (3,942) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 27       | 0.14          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 5        | 0.14          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 5        | 0.14          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 5        | 0.14          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 14       | 0.14          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 14       | 0.14          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 14       | 0.14          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 17       | 0.14          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 17       | 0.14          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 17       | 0.14          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 18       | 0.14          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 18       | 0.14          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 18       | 0.14          |
| (3,933) | 1:98:A:LYS:H | 1:19:A:ILE:HB   | 19       | 0.14          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,933) | 1:98:A:LYS:H | 1:19:A:ILE:HB   | 30       | 0.14          |
| (3,919) | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 36       | 0.14          |
| (3,916) | 1:37:A:ASP:H | 1:37:A:ASP:HA   | 1        | 0.14          |
| (3,900) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 4        | 0.14          |
| (3,889) | 1:80:A:SER:H | 1:43:A:TYR:HB3  | 4        | 0.14          |
| (3,889) | 1:80:A:SER:H | 1:43:A:TYR:HB3  | 11       | 0.14          |
| (3,889) | 1:80:A:SER:H | 1:43:A:TYR:HB3  | 32       | 0.14          |
| (3,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2   | 21       | 0.14          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 14       | 0.14          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 14       | 0.14          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 14       | 0.14          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 15       | 0.14          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 15       | 0.14          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 15       | 0.14          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 17       | 0.14          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 17       | 0.14          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 17       | 0.14          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 31       | 0.14          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 31       | 0.14          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 31       | 0.14          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 40       | 0.14          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 40       | 0.14          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 40       | 0.14          |
| (3,827) | 1:17:A:GLN:H | 1:17:A:GLN:HB2  | 8        | 0.14          |
| (3,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB   | 11       | 0.14          |
| (3,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB   | 14       | 0.14          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 1        | 0.14          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 1        | 0.14          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 1        | 0.14          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 2        | 0.14          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 2        | 0.14          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 2        | 0.14          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 4        | 0.14          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 4        | 0.14          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 4        | 0.14          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 9        | 0.14          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 9        | 0.14          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 9        | 0.14          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 10       | 0.14          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 10       | 0.14          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 10       | 0.14          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 15       | 0.14          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG12 | 15       | 0.14          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG13 | 15       | 0.14          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG11 | 18       | 0.14          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG12 | 18       | 0.14          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG13 | 18       | 0.14          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG11 | 22       | 0.14          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG12 | 22       | 0.14          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG13 | 22       | 0.14          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG11 | 26       | 0.14          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG12 | 26       | 0.14          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG13 | 26       | 0.14          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG11 | 27       | 0.14          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG12 | 27       | 0.14          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG13 | 27       | 0.14          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG11 | 31       | 0.14          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG12 | 31       | 0.14          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG13 | 31       | 0.14          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG11 | 32       | 0.14          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG12 | 32       | 0.14          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG13 | 32       | 0.14          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG11 | 35       | 0.14          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG12 | 35       | 0.14          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG13 | 35       | 0.14          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG11 | 39       | 0.14          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG12 | 39       | 0.14          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG13 | 39       | 0.14          |
| (3,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 26       | 0.14          |
| (3,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 19       | 0.14          |
| (3,683) | 1:23:A:GLU:H  | 1:22:A:SER:HB3  | 6        | 0.14          |
| (3,661) | 1:7:A:ALA:H   | 1:6:A:THR:HA    | 2        | 0.14          |
| (3,661) | 1:7:A:ALA:H   | 1:6:A:THR:HA    | 6        | 0.14          |
| (3,661) | 1:7:A:ALA:H   | 1:6:A:THR:HA    | 25       | 0.14          |
| (3,661) | 1:7:A:ALA:H   | 1:6:A:THR:HA    | 27       | 0.14          |
| (3,661) | 1:7:A:ALA:H   | 1:6:A:THR:HA    | 33       | 0.14          |
| (3,661) | 1:7:A:ALA:H   | 1:6:A:THR:HA    | 37       | 0.14          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 7        | 0.14          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 15       | 0.14          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 33       | 0.14          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 40       | 0.14          |
| (3,591) | 1:3:A:ASP:H   | 1:3:A:ASP:HA    | 9        | 0.14          |
| (3,589) | 1:93:A:SER:H  | 1:92:A:ARG:HG2  | 6        | 0.14          |
| (3,589) | 1:93:A:SER:H  | 1:92:A:ARG:HG2  | 29       | 0.14          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 5        | 0.14          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 5        | 0.14          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 5        | 0.14          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 8        | 0.14          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 8        | 0.14          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 8        | 0.14          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 24       | 0.14          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 24       | 0.14          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 24       | 0.14          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 31       | 0.14          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 31       | 0.14          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 31       | 0.14          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 40       | 0.14          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 40       | 0.14          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 40       | 0.14          |
| (3,560) | 1:47:A:THR:H | 1:47:A:THR:HA   | 2        | 0.14          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1  | 5        | 0.14          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2  | 5        | 0.14          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1  | 13       | 0.14          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2  | 13       | 0.14          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1  | 23       | 0.14          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2  | 23       | 0.14          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1  | 25       | 0.14          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2  | 25       | 0.14          |
| (3,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 10       | 0.14          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 7        | 0.14          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 11       | 0.14          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 19       | 0.14          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 34       | 0.14          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 10       | 0.14          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 12       | 0.14          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 16       | 0.14          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 24       | 0.14          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 25       | 0.14          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 26       | 0.14          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 27       | 0.14          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 30       | 0.14          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 32       | 0.14          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 40       | 0.14          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 16       | 0.14          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 24       | 0.14          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 26       | 0.14          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 32       | 0.14          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 40       | 0.14          |
| (3,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 10       | 0.14          |
| (3,419) | 1:69:A:HIS:H | 1:54:A:LYS:HA   | 12       | 0.14          |
| (3,410) | 1:96:A:GLU:H | 1:18:A:ASN:HD21 | 21       | 0.14          |
| (3,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD21 | 34       | 0.14          |
| (3,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD22 | 34       | 0.14          |
| (3,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD23 | 34       | 0.14          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 3        | 0.14          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 4        | 0.14          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 6        | 0.14          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 7        | 0.14          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 12       | 0.14          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 16       | 0.14          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 19       | 0.14          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 37       | 0.14          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 1        | 0.14          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 3        | 0.14          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 7        | 0.14          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 9        | 0.14          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 26       | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 1        | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 1        | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 1        | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 7        | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 7        | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 7        | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 17       | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 17       | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 17       | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 18       | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 18       | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 18       | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 19       | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 19       | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 19       | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 21       | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 21       | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 21       | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 24       | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 24       | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 24       | 0.14          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 33       | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 33       | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 33       | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 34       | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 34       | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 34       | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 35       | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 35       | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 35       | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 40       | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 40       | 0.14          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 40       | 0.14          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 1        | 0.14          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 1        | 0.14          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 1        | 0.14          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 4        | 0.14          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 4        | 0.14          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 4        | 0.14          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 10       | 0.14          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 10       | 0.14          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 10       | 0.14          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 16       | 0.14          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 16       | 0.14          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 16       | 0.14          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 27       | 0.14          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 27       | 0.14          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 27       | 0.14          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 29       | 0.14          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 29       | 0.14          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 29       | 0.14          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 34       | 0.14          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 34       | 0.14          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 34       | 0.14          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 39       | 0.14          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 39       | 0.14          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 39       | 0.14          |
| (3,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 1        | 0.14          |
| (3,368) | 1:18:A:ASN:H | 1:17:A:GLN:HB3  | 26       | 0.14          |
| (3,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD1  | 9        | 0.14          |
| (3,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD2  | 9        | 0.14          |
| (3,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 5        | 0.14          |
| (3,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 6        | 0.14          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 7        | 0.14          |
| (3,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 14       | 0.14          |
| (3,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 16       | 0.14          |
| (3,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 27       | 0.14          |
| (3,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 28       | 0.14          |
| (3,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 35       | 0.14          |
| (3,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 16       | 0.14          |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1  | 1        | 0.14          |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2  | 1        | 0.14          |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1  | 18       | 0.14          |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2  | 18       | 0.14          |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1  | 34       | 0.14          |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2  | 34       | 0.14          |
| (3,201) | 1:90:A:GLU:H | 1:89:A:GLY:HA2  | 6        | 0.14          |
| (3,201) | 1:90:A:GLU:H | 1:89:A:GLY:HA2  | 9        | 0.14          |
| (3,201) | 1:90:A:GLU:H | 1:89:A:GLY:HA2  | 28       | 0.14          |
| (3,198) | 1:90:A:GLU:H | 1:90:A:GLU:HB2  | 38       | 0.14          |
| (3,198) | 1:90:A:GLU:H | 1:90:A:GLU:HB2  | 39       | 0.14          |
| (3,138) | 1:39:A:ILE:H | 1:10:A:ILE:HD11 | 11       | 0.14          |
| (3,138) | 1:39:A:ILE:H | 1:10:A:ILE:HD12 | 11       | 0.14          |
| (3,138) | 1:39:A:ILE:H | 1:10:A:ILE:HD13 | 11       | 0.14          |
| (3,138) | 1:39:A:ILE:H | 1:10:A:ILE:HD11 | 36       | 0.14          |
| (3,138) | 1:39:A:ILE:H | 1:10:A:ILE:HD12 | 36       | 0.14          |
| (3,138) | 1:39:A:ILE:H | 1:10:A:ILE:HD13 | 36       | 0.14          |
| (3,59)  | 1:42:A:TRP:H | 1:41:A:THR:HB   | 7        | 0.14          |
| (3,50)  | 1:57:A:PHE:H | 1:57:A:PHE:HB3  | 2        | 0.14          |
| (3,50)  | 1:57:A:PHE:H | 1:57:A:PHE:HB3  | 3        | 0.14          |
| (3,50)  | 1:57:A:PHE:H | 1:57:A:PHE:HB3  | 5        | 0.14          |
| (3,50)  | 1:57:A:PHE:H | 1:57:A:PHE:HB3  | 8        | 0.14          |
| (3,50)  | 1:57:A:PHE:H | 1:57:A:PHE:HB3  | 10       | 0.14          |
| (3,50)  | 1:57:A:PHE:H | 1:57:A:PHE:HB3  | 11       | 0.14          |
| (3,50)  | 1:57:A:PHE:H | 1:57:A:PHE:HB3  | 12       | 0.14          |
| (3,50)  | 1:57:A:PHE:H | 1:57:A:PHE:HB3  | 14       | 0.14          |
| (3,50)  | 1:57:A:PHE:H | 1:57:A:PHE:HB3  | 16       | 0.14          |
| (3,50)  | 1:57:A:PHE:H | 1:57:A:PHE:HB3  | 20       | 0.14          |
| (3,50)  | 1:57:A:PHE:H | 1:57:A:PHE:HB3  | 21       | 0.14          |
| (3,50)  | 1:57:A:PHE:H | 1:57:A:PHE:HB3  | 24       | 0.14          |
| (3,50)  | 1:57:A:PHE:H | 1:57:A:PHE:HB3  | 25       | 0.14          |
| (3,50)  | 1:57:A:PHE:H | 1:57:A:PHE:HB3  | 26       | 0.14          |
| (3,50)  | 1:57:A:PHE:H | 1:57:A:PHE:HB3  | 27       | 0.14          |
| (3,50)  | 1:57:A:PHE:H | 1:57:A:PHE:HB3  | 29       | 0.14          |
| (3,50)  | 1:57:A:PHE:H | 1:57:A:PHE:HB3  | 31       | 0.14          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,50)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 32       | 0.14          |
| (3,50)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 33       | 0.14          |
| (3,50)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 37       | 0.14          |
| (3,50)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 40       | 0.14          |
| (3,39)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3  | 21       | 0.14          |
| (3,39)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3  | 31       | 0.14          |
| (3,39)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3  | 40       | 0.14          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 4        | 0.14          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 4        | 0.14          |
| (1,3212) | 1:65:A:TYR:HE1 | 1:58:A:ARG:HB3  | 10       | 0.14          |
| (1,3212) | 1:65:A:TYR:HE2 | 1:58:A:ARG:HB3  | 10       | 0.14          |
| (1,3211) | 1:69:A:HIS:HE1 | 1:67:A:THR:HB   | 30       | 0.14          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 21       | 0.14          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 21       | 0.14          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 21       | 0.14          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 21       | 0.14          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 21       | 0.14          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 21       | 0.14          |
| (1,3197) | 1:42:A:TRP:HZ2 | 1:30:A:GLU:HA   | 12       | 0.14          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 5        | 0.14          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 5        | 0.14          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 5        | 0.14          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 5        | 0.14          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 8        | 0.14          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 8        | 0.14          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 8        | 0.14          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 8        | 0.14          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 33       | 0.14          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 33       | 0.14          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 33       | 0.14          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 33       | 0.14          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 15       | 0.14          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 36       | 0.14          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 16       | 0.14          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 16       | 0.14          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 16       | 0.14          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 28       | 0.14          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 28       | 0.14          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 28       | 0.14          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 33       | 0.14          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 33       | 0.14          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 33       | 0.14          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1 | 39       | 0.14          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2 | 39       | 0.14          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3 | 39       | 0.14          |
| (1,3169) | 1:69:A:HIS:HD2 | 1:69:A:HIS:HB3 | 15       | 0.14          |
| (1,3169) | 1:69:A:HIS:HD2 | 1:69:A:HIS:HB3 | 17       | 0.14          |
| (1,3169) | 1:69:A:HIS:HD2 | 1:69:A:HIS:HB3 | 28       | 0.14          |
| (1,3169) | 1:69:A:HIS:HD2 | 1:69:A:HIS:HB3 | 29       | 0.14          |
| (1,3158) | 1:42:A:TRP:HD1 | 1:41:A:THR:HA  | 6        | 0.14          |
| (1,3158) | 1:42:A:TRP:HD1 | 1:41:A:THR:HA  | 11       | 0.14          |
| (1,3137) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3 | 7        | 0.14          |
| (1,3137) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3 | 7        | 0.14          |
| (1,3137) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3 | 15       | 0.14          |
| (1,3137) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3 | 15       | 0.14          |
| (1,3137) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3 | 16       | 0.14          |
| (1,3137) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3 | 16       | 0.14          |
| (1,3137) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3 | 20       | 0.14          |
| (1,3137) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3 | 20       | 0.14          |
| (1,3137) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3 | 35       | 0.14          |
| (1,3137) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3 | 35       | 0.14          |
| (1,3137) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3 | 36       | 0.14          |
| (1,3137) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3 | 36       | 0.14          |
| (1,3137) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3 | 39       | 0.14          |
| (1,3137) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3 | 39       | 0.14          |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 7        | 0.14          |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 7        | 0.14          |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 10       | 0.14          |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 10       | 0.14          |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 21       | 0.14          |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 21       | 0.14          |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 24       | 0.14          |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 24       | 0.14          |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 33       | 0.14          |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 33       | 0.14          |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 37       | 0.14          |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 37       | 0.14          |
| (1,3133) | 1:65:A:TYR:HE1 | 1:60:A:ASP:HB3 | 13       | 0.14          |
| (1,3133) | 1:65:A:TYR:HE2 | 1:60:A:ASP:HB3 | 13       | 0.14          |
| (1,3132) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB2 | 23       | 0.14          |
| (1,3132) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB2 | 23       | 0.14          |
| (1,3131) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3 | 15       | 0.14          |
| (1,3131) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3 | 15       | 0.14          |
| (1,3131) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3 | 32       | 0.14          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3131) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3  | 32       | 0.14          |
| (1,3131) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3  | 39       | 0.14          |
| (1,3131) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3  | 39       | 0.14          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 1        | 0.14          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 1        | 0.14          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 7        | 0.14          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 7        | 0.14          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 22       | 0.14          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 22       | 0.14          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 27       | 0.14          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 27       | 0.14          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 1        | 0.14          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 1        | 0.14          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 7        | 0.14          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 7        | 0.14          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 22       | 0.14          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 22       | 0.14          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 27       | 0.14          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 27       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 3        | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 3        | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 3        | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 3        | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 3        | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 3        | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 11       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 11       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 11       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 11       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 11       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 11       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 14       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 14       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 14       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 14       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 14       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 14       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 15       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 15       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 15       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 15       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 15       | 0.14          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 15       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 21       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 21       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 21       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 21       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 21       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 21       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 22       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 22       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 22       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 22       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 22       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 22       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 23       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 23       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 23       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 23       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 23       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 23       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 25       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 25       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 25       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 25       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 25       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 25       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 27       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 27       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 27       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 27       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 27       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 27       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 30       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 30       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 30       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 30       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 30       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 30       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 38       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 38       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 38       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 38       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 38       | 0.14          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 38       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 39       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 39       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 39       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 39       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 39       | 0.14          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 39       | 0.14          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 23       | 0.14          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 23       | 0.14          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 23       | 0.14          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 23       | 0.14          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 23       | 0.14          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 23       | 0.14          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 34       | 0.14          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 34       | 0.14          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 34       | 0.14          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 34       | 0.14          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 34       | 0.14          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 34       | 0.14          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 19       | 0.14          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 19       | 0.14          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 19       | 0.14          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 19       | 0.14          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 25       | 0.14          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 25       | 0.14          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 25       | 0.14          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 25       | 0.14          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 31       | 0.14          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 31       | 0.14          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 31       | 0.14          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 31       | 0.14          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 4        | 0.14          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 4        | 0.14          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 4        | 0.14          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 4        | 0.14          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 4        | 0.14          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 4        | 0.14          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 8        | 0.14          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 8        | 0.14          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 8        | 0.14          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 8        | 0.14          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 8        | 0.14          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 8        | 0.14          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 31       | 0.14          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 31       | 0.14          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 31       | 0.14          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 31       | 0.14          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 31       | 0.14          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 31       | 0.14          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 33       | 0.14          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 33       | 0.14          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 33       | 0.14          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 33       | 0.14          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 33       | 0.14          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 33       | 0.14          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 40       | 0.14          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 40       | 0.14          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 40       | 0.14          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 40       | 0.14          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 40       | 0.14          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 40       | 0.14          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 1        | 0.14          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 1        | 0.14          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 1        | 0.14          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 2        | 0.14          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 2        | 0.14          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 2        | 0.14          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 7        | 0.14          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 7        | 0.14          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 7        | 0.14          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 15       | 0.14          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 15       | 0.14          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 15       | 0.14          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 32       | 0.14          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 32       | 0.14          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 32       | 0.14          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 34       | 0.14          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 34       | 0.14          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 34       | 0.14          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 37       | 0.14          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 37       | 0.14          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 37       | 0.14          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 40       | 0.14          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 40       | 0.14          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 40       | 0.14          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 11       | 0.14          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 11       | 0.14          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 12       | 0.14          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 12       | 0.14          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 21       | 0.14          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 21       | 0.14          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 23       | 0.14          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 23       | 0.14          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 25       | 0.14          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 25       | 0.14          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 34       | 0.14          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 34       | 0.14          |
| (1,3047) | 1:57:A:PHE:HB3 | 1:42:A:TRP:HE1  | 9        | 0.14          |
| (1,3040) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG21 | 15       | 0.14          |
| (1,3040) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG22 | 15       | 0.14          |
| (1,3040) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG23 | 15       | 0.14          |
| (1,3033) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE1  | 4        | 0.14          |
| (1,3033) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE2  | 4        | 0.14          |
| (1,3033) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE1  | 9        | 0.14          |
| (1,3033) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE2  | 9        | 0.14          |
| (1,3033) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE1  | 39       | 0.14          |
| (1,3033) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE2  | 39       | 0.14          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 1        | 0.14          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 1        | 0.14          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 19       | 0.14          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 19       | 0.14          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 28       | 0.14          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 28       | 0.14          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 5        | 0.14          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 5        | 0.14          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 5        | 0.14          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 7        | 0.14          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 7        | 0.14          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 7        | 0.14          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 26       | 0.14          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 26       | 0.14          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 26       | 0.14          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 32       | 0.14          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 32       | 0.14          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 32       | 0.14          |
| (1,3011) | 1:30:A:GLU:HB2 | 1:14:A:LYS:HE2  | 4        | 0.14          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,3011) | 1:30:A:GLU:HB2 | 1:14:A:LYS:HE2 | 24       | 0.14          |
| (1,3011) | 1:30:A:GLU:HB2 | 1:14:A:LYS:HE2 | 28       | 0.14          |
| (1,3011) | 1:30:A:GLU:HB2 | 1:14:A:LYS:HE2 | 33       | 0.14          |
| (1,2996) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3 | 5        | 0.14          |
| (1,2996) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3 | 39       | 0.14          |
| (1,2996) | 1:15:A:ARG:HG2 | 1:93:A:SER:HB3 | 40       | 0.14          |
| (1,2974) | 1:65:A:TYR:HA  | 1:42:A:TRP:HZ2 | 28       | 0.14          |
| (1,2962) | 1:44:A:LYS:HE2 | 1:44:A:LYS:HG3 | 2        | 0.14          |
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 15       | 0.14          |
| (1,2949) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 6        | 0.14          |
| (1,2949) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 15       | 0.14          |
| (1,2949) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 26       | 0.14          |
| (1,2949) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 29       | 0.14          |
| (1,2949) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 30       | 0.14          |
| (1,2949) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 36       | 0.14          |
| (1,2942) | 1:90:A:GLU:HA  | 1:84:A:ARG:HA  | 1        | 0.14          |
| (1,2942) | 1:90:A:GLU:HA  | 1:84:A:ARG:HA  | 5        | 0.14          |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1 | 7        | 0.14          |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2 | 7        | 0.14          |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1 | 15       | 0.14          |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2 | 15       | 0.14          |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1 | 16       | 0.14          |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2 | 16       | 0.14          |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1 | 20       | 0.14          |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2 | 20       | 0.14          |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1 | 35       | 0.14          |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2 | 35       | 0.14          |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1 | 36       | 0.14          |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2 | 36       | 0.14          |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1 | 39       | 0.14          |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2 | 39       | 0.14          |
| (1,2931) | 1:26:A:SER:HA  | 1:70:A:ASN:H   | 11       | 0.14          |
| (1,2931) | 1:26:A:SER:HA  | 1:70:A:ASN:H   | 30       | 0.14          |
| (1,2929) | 1:17:A:GLN:HG2 | 1:17:A:GLN:H   | 37       | 0.14          |
| (1,2903) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD2 | 1        | 0.14          |
| (1,2903) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD2 | 6        | 0.14          |
| (1,2903) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD2 | 8        | 0.14          |
| (1,2903) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD2 | 9        | 0.14          |
| (1,2903) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD2 | 19       | 0.14          |
| (1,2903) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD2 | 23       | 0.14          |
| (1,2903) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD2 | 24       | 0.14          |
| (1,2903) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD2 | 25       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2903) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 26       | 0.14          |
| (1,2903) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 30       | 0.14          |
| (1,2903) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 31       | 0.14          |
| (1,2903) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 32       | 0.14          |
| (1,2903) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 33       | 0.14          |
| (1,2903) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 34       | 0.14          |
| (1,2903) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 35       | 0.14          |
| (1,2903) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 37       | 0.14          |
| (1,2903) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 39       | 0.14          |
| (1,2903) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 40       | 0.14          |
| (1,2859) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 14       | 0.14          |
| (1,2859) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 17       | 0.14          |
| (1,2859) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 18       | 0.14          |
| (1,2859) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 34       | 0.14          |
| (1,2859) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 35       | 0.14          |
| (1,2859) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 39       | 0.14          |
| (1,2859) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 40       | 0.14          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 7        | 0.14          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 2        | 0.14          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 4        | 0.14          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 6        | 0.14          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 11       | 0.14          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 29       | 0.14          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 31       | 0.14          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 33       | 0.14          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 34       | 0.14          |
| (1,2754) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 4        | 0.14          |
| (1,2754) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 19       | 0.14          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H    | 3        | 0.14          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H    | 4        | 0.14          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H    | 6        | 0.14          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H    | 7        | 0.14          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H    | 12       | 0.14          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H    | 16       | 0.14          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H    | 19       | 0.14          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H    | 37       | 0.14          |
| (1,2715) | 1:48:A:GLU:HA   | 1:49:A:LEU:HG   | 16       | 0.14          |
| (1,2699) | 1:23:A:GLU:HA   | 1:24:A:HIS:HA   | 6        | 0.14          |
| (1,2686) | 1:8:A:GLU:HB3   | 1:8:A:GLU:HG2   | 6        | 0.14          |
| (1,2686) | 1:8:A:GLU:HB3   | 1:8:A:GLU:HG2   | 10       | 0.14          |
| (1,2686) | 1:8:A:GLU:HB3   | 1:8:A:GLU:HG2   | 20       | 0.14          |
| (1,2686) | 1:8:A:GLU:HB3   | 1:8:A:GLU:HG2   | 26       | 0.14          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,2686) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2  | 30       | 0.14          |
| (1,2686) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2  | 33       | 0.14          |
| (1,2686) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2  | 34       | 0.14          |
| (1,2686) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2  | 36       | 0.14          |
| (1,2686) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2  | 37       | 0.14          |
| (1,2675) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 2        | 0.14          |
| (1,2675) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 8        | 0.14          |
| (1,2675) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 15       | 0.14          |
| (1,2675) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 18       | 0.14          |
| (1,2675) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 20       | 0.14          |
| (1,2675) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 23       | 0.14          |
| (1,2675) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 24       | 0.14          |
| (1,2675) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 27       | 0.14          |
| (1,2675) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 31       | 0.14          |
| (1,2675) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 32       | 0.14          |
| (1,2675) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 37       | 0.14          |
| (1,2675) | 1:25:A:GLN:HG3 | 1:26:A:SER:H   | 40       | 0.14          |
| (1,2649) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H   | 1        | 0.14          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3  | 28       | 0.14          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3  | 30       | 0.14          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3  | 31       | 0.14          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3  | 34       | 0.14          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3  | 38       | 0.14          |
| (1,2597) | 1:36:A:ASP:HB3 | 1:37:A:ASP:H   | 36       | 0.14          |
| (1,2550) | 1:92:A:ARG:HA  | 1:83:A:ALA:H   | 19       | 0.14          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 4        | 0.14          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 6        | 0.14          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 7        | 0.14          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA  | 15       | 0.14          |
| (1,2537) | 1:73:A:PRO:HG3 | 1:73:A:PRO:HA  | 24       | 0.14          |
| (1,2537) | 1:73:A:PRO:HG3 | 1:73:A:PRO:HA  | 36       | 0.14          |
| (1,2537) | 1:73:A:PRO:HG3 | 1:73:A:PRO:HA  | 40       | 0.14          |
| (1,2511) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 14       | 0.14          |
| (1,2511) | 1:46:A:PRO:HB3 | 1:46:A:PRO:HD2 | 16       | 0.14          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2  | 8        | 0.14          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2  | 17       | 0.14          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA   | 3        | 0.14          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA   | 5        | 0.14          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA   | 6        | 0.14          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA   | 7        | 0.14          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA   | 12       | 0.14          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA   | 14       | 0.14          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA   | 28       | 0.14          |
| (1,2431) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 16       | 0.14          |
| (1,2431) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 27       | 0.14          |
| (1,2431) | 1:82:A:ILE:HB  | 1:41:A:THR:H   | 38       | 0.14          |
| (1,2416) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA   | 19       | 0.14          |
| (1,2416) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA   | 21       | 0.14          |
| (1,2416) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA   | 24       | 0.14          |
| (1,2416) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA   | 25       | 0.14          |
| (1,2416) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA   | 35       | 0.14          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 1        | 0.14          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 7        | 0.14          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 10       | 0.14          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 26       | 0.14          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 27       | 0.14          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2 | 34       | 0.14          |
| (1,2403) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 5        | 0.14          |
| (1,2403) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 5        | 0.14          |
| (1,2403) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 5        | 0.14          |
| (1,2403) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 15       | 0.14          |
| (1,2403) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 15       | 0.14          |
| (1,2403) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 15       | 0.14          |
| (1,2403) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 31       | 0.14          |
| (1,2403) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 31       | 0.14          |
| (1,2403) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 31       | 0.14          |
| (1,2403) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 35       | 0.14          |
| (1,2403) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 35       | 0.14          |
| (1,2403) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 35       | 0.14          |
| (1,2403) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 37       | 0.14          |
| (1,2403) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 37       | 0.14          |
| (1,2403) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 37       | 0.14          |
| (1,2403) | 1:66:A:MET:HE1 | 1:42:A:TRP:H   | 38       | 0.14          |
| (1,2403) | 1:66:A:MET:HE2 | 1:42:A:TRP:H   | 38       | 0.14          |
| (1,2403) | 1:66:A:MET:HE3 | 1:42:A:TRP:H   | 38       | 0.14          |
| (1,2402) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 1        | 0.14          |
| (1,2402) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 1        | 0.14          |
| (1,2402) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 1        | 0.14          |
| (1,2402) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 16       | 0.14          |
| (1,2402) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 16       | 0.14          |
| (1,2402) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 16       | 0.14          |
| (1,2402) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ  | 19       | 0.14          |
| (1,2402) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ  | 19       | 0.14          |
| (1,2402) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ  | 19       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2287) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 1        | 0.14          |
| (1,2287) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 10       | 0.14          |
| (1,2287) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 11       | 0.14          |
| (1,2287) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 15       | 0.14          |
| (1,2287) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 20       | 0.14          |
| (1,2287) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 21       | 0.14          |
| (1,2287) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 23       | 0.14          |
| (1,2287) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 24       | 0.14          |
| (1,2287) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 26       | 0.14          |
| (1,2287) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 27       | 0.14          |
| (1,2287) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 30       | 0.14          |
| (1,2287) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 32       | 0.14          |
| (1,2287) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 36       | 0.14          |
| (1,2287) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 39       | 0.14          |
| (1,2287) | 1:96:A:GLU:HG2  | 1:96:A:GLU:H    | 40       | 0.14          |
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG21 | 11       | 0.14          |
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG22 | 11       | 0.14          |
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG23 | 11       | 0.14          |
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG21 | 34       | 0.14          |
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG22 | 34       | 0.14          |
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG23 | 34       | 0.14          |
| (1,2237) | 1:18:A:ASN:HB2  | 1:18:A:ASN:H    | 7        | 0.14          |
| (1,2237) | 1:18:A:ASN:HB2  | 1:18:A:ASN:H    | 22       | 0.14          |
| (1,2237) | 1:18:A:ASN:HB2  | 1:18:A:ASN:H    | 23       | 0.14          |
| (1,2237) | 1:18:A:ASN:HB2  | 1:18:A:ASN:H    | 31       | 0.14          |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD11 | 27       | 0.14          |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD12 | 27       | 0.14          |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD13 | 27       | 0.14          |
| (1,2145) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 13       | 0.14          |
| (1,2145) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 19       | 0.14          |
| (1,2145) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 34       | 0.14          |
| (1,2145) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 39       | 0.14          |
| (1,2136) | 1:67:A:THR:HB   | 1:56:A:ASN:HB2  | 4        | 0.14          |
| (1,2099) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HA   | 11       | 0.14          |
| (1,2099) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HA   | 11       | 0.14          |
| (1,2099) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HA   | 11       | 0.14          |
| (1,2099) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HA   | 22       | 0.14          |
| (1,2099) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HA   | 22       | 0.14          |
| (1,2099) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HA   | 22       | 0.14          |
| (1,2099) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HA   | 31       | 0.14          |
| (1,2099) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HA   | 31       | 0.14          |
| (1,2099) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HA   | 31       | 0.14          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2 | 2        | 0.14          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2 | 2        | 0.14          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2 | 2        | 0.14          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2 | 16       | 0.14          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2 | 16       | 0.14          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2 | 16       | 0.14          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2 | 28       | 0.14          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2 | 28       | 0.14          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2 | 28       | 0.14          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2 | 35       | 0.14          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2 | 35       | 0.14          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2 | 35       | 0.14          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2 | 39       | 0.14          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2 | 39       | 0.14          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2 | 39       | 0.14          |
| (1,2093) | 1:88:A:ARG:HD3  | 1:7:A:ALA:HA   | 20       | 0.14          |
| (1,2087) | 1:85:A:LEU:HD11 | 1:39:A:ILE:H   | 8        | 0.14          |
| (1,2087) | 1:85:A:LEU:HD12 | 1:39:A:ILE:H   | 8        | 0.14          |
| (1,2087) | 1:85:A:LEU:HD13 | 1:39:A:ILE:H   | 8        | 0.14          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1 | 6        | 0.14          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2 | 6        | 0.14          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1 | 6        | 0.14          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2 | 6        | 0.14          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1 | 6        | 0.14          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2 | 6        | 0.14          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1 | 11       | 0.14          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2 | 11       | 0.14          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1 | 11       | 0.14          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2 | 11       | 0.14          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1 | 11       | 0.14          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2 | 11       | 0.14          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1 | 27       | 0.14          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2 | 27       | 0.14          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1 | 27       | 0.14          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2 | 27       | 0.14          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1 | 27       | 0.14          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2 | 27       | 0.14          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1 | 34       | 0.14          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2 | 34       | 0.14          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1 | 34       | 0.14          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2 | 34       | 0.14          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1 | 34       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2  | 34       | 0.14          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1  | 38       | 0.14          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2  | 38       | 0.14          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1  | 38       | 0.14          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2  | 38       | 0.14          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1  | 38       | 0.14          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2  | 38       | 0.14          |
| (1,2068) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 29       | 0.14          |
| (1,2068) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 29       | 0.14          |
| (1,2068) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 29       | 0.14          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3  | 20       | 0.14          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3  | 20       | 0.14          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3  | 20       | 0.14          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD21 | 5        | 0.14          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD22 | 5        | 0.14          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD23 | 5        | 0.14          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD21 | 5        | 0.14          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD22 | 5        | 0.14          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD23 | 5        | 0.14          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD21 | 5        | 0.14          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD22 | 5        | 0.14          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD23 | 5        | 0.14          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD21 | 17       | 0.14          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD22 | 17       | 0.14          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD23 | 17       | 0.14          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD21 | 17       | 0.14          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD22 | 17       | 0.14          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD23 | 17       | 0.14          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD21 | 17       | 0.14          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD22 | 17       | 0.14          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD23 | 17       | 0.14          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1  | 16       | 0.14          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2  | 16       | 0.14          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1  | 16       | 0.14          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2  | 16       | 0.14          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1  | 16       | 0.14          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2  | 16       | 0.14          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1  | 19       | 0.14          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2  | 19       | 0.14          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1  | 19       | 0.14          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2  | 19       | 0.14          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1  | 19       | 0.14          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 19       | 0.14          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 25       | 0.14          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 25       | 0.14          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 25       | 0.14          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 37       | 0.14          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 37       | 0.14          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 37       | 0.14          |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 2        | 0.14          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 2        | 0.14          |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 2        | 0.14          |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 8        | 0.14          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 8        | 0.14          |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 8        | 0.14          |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 17       | 0.14          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 17       | 0.14          |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 17       | 0.14          |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 22       | 0.14          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 22       | 0.14          |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 22       | 0.14          |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 28       | 0.14          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 28       | 0.14          |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 28       | 0.14          |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 40       | 0.14          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 40       | 0.14          |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 40       | 0.14          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 1        | 0.14          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 1        | 0.14          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 1        | 0.14          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 1        | 0.14          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 1        | 0.14          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 1        | 0.14          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 11       | 0.14          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 11       | 0.14          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 11       | 0.14          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 11       | 0.14          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 11       | 0.14          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 11       | 0.14          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 14       | 0.14          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 14       | 0.14          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 14       | 0.14          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 14       | 0.14          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 14       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2  | 14       | 0.14          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1  | 17       | 0.14          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2  | 17       | 0.14          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3  | 17       | 0.14          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1  | 17       | 0.14          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2  | 17       | 0.14          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3  | 17       | 0.14          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1  | 17       | 0.14          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2  | 17       | 0.14          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3  | 17       | 0.14          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1  | 20       | 0.14          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2  | 20       | 0.14          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3  | 20       | 0.14          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1  | 20       | 0.14          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2  | 20       | 0.14          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3  | 20       | 0.14          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1  | 20       | 0.14          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2  | 20       | 0.14          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3  | 20       | 0.14          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 5        | 0.14          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 6        | 0.14          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 7        | 0.14          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 14       | 0.14          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 16       | 0.14          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 27       | 0.14          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 28       | 0.14          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 35       | 0.14          |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 18       | 0.14          |
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 18       | 0.14          |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 18       | 0.14          |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 20       | 0.14          |
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 20       | 0.14          |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 20       | 0.14          |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 32       | 0.14          |
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 32       | 0.14          |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 32       | 0.14          |
| (1,1990) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 9        | 0.14          |
| (1,1990) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 9        | 0.14          |
| (1,1990) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 9        | 0.14          |
| (1,1990) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 28       | 0.14          |
| (1,1990) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 28       | 0.14          |
| (1,1990) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 28       | 0.14          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA  | 14       | 0.14          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA  | 23       | 0.14          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA  | 25       | 0.14          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA  | 28       | 0.14          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA  | 30       | 0.14          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA  | 37       | 0.14          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA  | 39       | 0.14          |
| (1,1956) | 1:72:A:THR:HG21 | 1:74:A:ASP:HB3 | 11       | 0.14          |
| (1,1956) | 1:72:A:THR:HG22 | 1:74:A:ASP:HB3 | 11       | 0.14          |
| (1,1956) | 1:72:A:THR:HG23 | 1:74:A:ASP:HB3 | 11       | 0.14          |
| (1,1956) | 1:72:A:THR:HG21 | 1:74:A:ASP:HB3 | 36       | 0.14          |
| (1,1956) | 1:72:A:THR:HG22 | 1:74:A:ASP:HB3 | 36       | 0.14          |
| (1,1956) | 1:72:A:THR:HG23 | 1:74:A:ASP:HB3 | 36       | 0.14          |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 4        | 0.14          |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 4        | 0.14          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 4        | 0.14          |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 14       | 0.14          |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 14       | 0.14          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 14       | 0.14          |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 22       | 0.14          |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 22       | 0.14          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 22       | 0.14          |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 32       | 0.14          |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 32       | 0.14          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 32       | 0.14          |
| (1,1903) | 1:66:A:MET:HE1  | 1:79:A:TYR:HA  | 7        | 0.14          |
| (1,1903) | 1:66:A:MET:HE2  | 1:79:A:TYR:HA  | 7        | 0.14          |
| (1,1903) | 1:66:A:MET:HE3  | 1:79:A:TYR:HA  | 7        | 0.14          |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 5        | 0.14          |
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 5        | 0.14          |
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 5        | 0.14          |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 9        | 0.14          |
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 9        | 0.14          |
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 9        | 0.14          |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 13       | 0.14          |
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 13       | 0.14          |
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 13       | 0.14          |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 14       | 0.14          |
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 14       | 0.14          |
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 14       | 0.14          |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 16       | 0.14          |
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 16       | 0.14          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 16       | 0.14          |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 23       | 0.14          |
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 23       | 0.14          |
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 23       | 0.14          |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 32       | 0.14          |
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 32       | 0.14          |
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 32       | 0.14          |
| (1,1896) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3 | 10       | 0.14          |
| (1,1896) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3 | 10       | 0.14          |
| (1,1896) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3 | 10       | 0.14          |
| (1,1896) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3 | 37       | 0.14          |
| (1,1896) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3 | 37       | 0.14          |
| (1,1896) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3 | 37       | 0.14          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H   | 6        | 0.14          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H   | 6        | 0.14          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H   | 6        | 0.14          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H   | 17       | 0.14          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H   | 17       | 0.14          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H   | 17       | 0.14          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H   | 20       | 0.14          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H   | 20       | 0.14          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H   | 20       | 0.14          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H   | 25       | 0.14          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H   | 25       | 0.14          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H   | 25       | 0.14          |
| (1,1894) | 1:41:A:THR:HG21 | 1:41:A:THR:H   | 28       | 0.14          |
| (1,1894) | 1:41:A:THR:HG22 | 1:41:A:THR:H   | 28       | 0.14          |
| (1,1894) | 1:41:A:THR:HG23 | 1:41:A:THR:H   | 28       | 0.14          |
| (1,1861) | 1:7:A:ALA:HB1   | 1:88:A:ARG:HA  | 16       | 0.14          |
| (1,1861) | 1:7:A:ALA:HB2   | 1:88:A:ARG:HA  | 16       | 0.14          |
| (1,1861) | 1:7:A:ALA:HB3   | 1:88:A:ARG:HA  | 16       | 0.14          |
| (1,1861) | 1:7:A:ALA:HB1   | 1:88:A:ARG:HA  | 37       | 0.14          |
| (1,1861) | 1:7:A:ALA:HB2   | 1:88:A:ARG:HA  | 37       | 0.14          |
| (1,1861) | 1:7:A:ALA:HB3   | 1:88:A:ARG:HA  | 37       | 0.14          |
| (1,1853) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 17       | 0.14          |
| (1,1853) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 17       | 0.14          |
| (1,1853) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 17       | 0.14          |
| (1,1853) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 20       | 0.14          |
| (1,1853) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 20       | 0.14          |
| (1,1853) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 20       | 0.14          |
| (1,1811) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 3        | 0.14          |
| (1,1811) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 4        | 0.14          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 5        | 0.14          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 7        | 0.14          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 10       | 0.14          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 13       | 0.14          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 14       | 0.14          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 15       | 0.14          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 17       | 0.14          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 19       | 0.14          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 20       | 0.14          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 21       | 0.14          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 22       | 0.14          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 23       | 0.14          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 24       | 0.14          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 25       | 0.14          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 29       | 0.14          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 30       | 0.14          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 31       | 0.14          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 32       | 0.14          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 34       | 0.14          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 35       | 0.14          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 36       | 0.14          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 38       | 0.14          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 39       | 0.14          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 40       | 0.14          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 15       | 0.14          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 18       | 0.14          |
| (1,1810) | 1:98:A:LYS:HD3 | 1:98:A:LYS:HG3  | 27       | 0.14          |
| (1,1803) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 15       | 0.14          |
| (1,1717) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG11 | 2        | 0.14          |
| (1,1717) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG12 | 2        | 0.14          |
| (1,1717) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG13 | 2        | 0.14          |
| (1,1717) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG11 | 2        | 0.14          |
| (1,1717) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG12 | 2        | 0.14          |
| (1,1717) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG13 | 2        | 0.14          |
| (1,1717) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG11 | 2        | 0.14          |
| (1,1717) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG12 | 2        | 0.14          |
| (1,1717) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG13 | 2        | 0.14          |
| (1,1717) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG11 | 20       | 0.14          |
| (1,1717) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG12 | 20       | 0.14          |
| (1,1717) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG13 | 20       | 0.14          |
| (1,1717) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG11 | 20       | 0.14          |
| (1,1717) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG12 | 20       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 20       | 0.14          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 20       | 0.14          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 20       | 0.14          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 20       | 0.14          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG11 | 25       | 0.14          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG12 | 25       | 0.14          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG13 | 25       | 0.14          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG11 | 25       | 0.14          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG12 | 25       | 0.14          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 25       | 0.14          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 25       | 0.14          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 25       | 0.14          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 25       | 0.14          |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 4        | 0.14          |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 4        | 0.14          |
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 4        | 0.14          |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 26       | 0.14          |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 26       | 0.14          |
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 26       | 0.14          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 3        | 0.14          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 3        | 0.14          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 3        | 0.14          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 3        | 0.14          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 3        | 0.14          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 3        | 0.14          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 3        | 0.14          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 3        | 0.14          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 3        | 0.14          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 8        | 0.14          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 8        | 0.14          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 8        | 0.14          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 8        | 0.14          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 8        | 0.14          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 8        | 0.14          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 8        | 0.14          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 8        | 0.14          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 8        | 0.14          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 14       | 0.14          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 14       | 0.14          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 14       | 0.14          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 14       | 0.14          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 14       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 14       | 0.14          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 14       | 0.14          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 14       | 0.14          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 14       | 0.14          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 26       | 0.14          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 26       | 0.14          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 26       | 0.14          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 26       | 0.14          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 26       | 0.14          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 26       | 0.14          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 26       | 0.14          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 26       | 0.14          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 26       | 0.14          |
| (1,1679) | 1:85:A:LEU:HD11 | 1:35:A:PHE:HD1  | 5        | 0.14          |
| (1,1679) | 1:85:A:LEU:HD11 | 1:35:A:PHE:HD2  | 5        | 0.14          |
| (1,1679) | 1:85:A:LEU:HD12 | 1:35:A:PHE:HD1  | 5        | 0.14          |
| (1,1679) | 1:85:A:LEU:HD12 | 1:35:A:PHE:HD2  | 5        | 0.14          |
| (1,1679) | 1:85:A:LEU:HD13 | 1:35:A:PHE:HD1  | 5        | 0.14          |
| (1,1679) | 1:85:A:LEU:HD13 | 1:35:A:PHE:HD2  | 5        | 0.14          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 32       | 0.14          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 32       | 0.14          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 32       | 0.14          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 32       | 0.14          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 32       | 0.14          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 32       | 0.14          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 32       | 0.14          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 32       | 0.14          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 32       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 1        | 0.14          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 1        | 0.14          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 1        | 0.14          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 5        | 0.14          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 5        | 0.14          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 5        | 0.14          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 8        | 0.14          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 8        | 0.14          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 8        | 0.14          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 11       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 11       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 11       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 13       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 13       | 0.14          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 13       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H   | 21       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H   | 21       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 21       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H   | 22       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H   | 22       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 22       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H   | 24       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H   | 24       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 24       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H   | 27       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H   | 27       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 27       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H   | 30       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H   | 30       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 30       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H   | 31       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H   | 31       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 31       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H   | 32       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H   | 32       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 32       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H   | 34       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H   | 34       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 34       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H   | 38       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H   | 38       | 0.14          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 38       | 0.14          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2 | 1        | 0.14          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 1        | 0.14          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 1        | 0.14          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2 | 14       | 0.14          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 14       | 0.14          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 14       | 0.14          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2 | 22       | 0.14          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 22       | 0.14          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 22       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 3        | 0.14          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 3        | 0.14          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 3        | 0.14          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 3        | 0.14          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 3        | 0.14          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 3        | 0.14          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 11       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 11       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 11       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 11       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 11       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 11       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 14       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 14       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 14       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 14       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 14       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 14       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 15       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 15       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 15       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 15       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 15       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 15       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 21       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 21       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 21       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 21       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 21       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 21       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 22       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 22       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 22       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 22       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 22       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 22       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 23       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 23       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 23       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 23       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 23       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 23       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 25       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 25       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 25       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 25       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 25       | 0.14          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 25       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 27       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 27       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 27       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 27       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 27       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 27       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 30       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 30       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 30       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 30       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 30       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 30       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 38       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 38       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 38       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 38       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 38       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 38       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 39       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 39       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 39       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 39       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 39       | 0.14          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 39       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 2        | 0.14          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 2        | 0.14          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 2        | 0.14          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 2        | 0.14          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 2        | 0.14          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 2        | 0.14          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 22       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 22       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 22       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 22       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 22       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 22       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 24       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 24       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 24       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 24       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 24       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 24       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 25       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 25       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 25       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 25       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 25       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 25       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 34       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 34       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 34       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 34       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 34       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 34       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 35       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 35       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 35       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 35       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 35       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 35       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 36       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 36       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 36       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 36       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 36       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 36       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 38       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 38       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 38       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 38       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 38       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 38       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 39       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 39       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 39       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 39       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 39       | 0.14          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 39       | 0.14          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 9        | 0.14          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 9        | 0.14          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 9        | 0.14          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 10       | 0.14          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 10       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 10       | 0.14          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 16       | 0.14          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 16       | 0.14          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 16       | 0.14          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 17       | 0.14          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 17       | 0.14          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 17       | 0.14          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 19       | 0.14          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 19       | 0.14          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 19       | 0.14          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 28       | 0.14          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 28       | 0.14          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 28       | 0.14          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 3        | 0.14          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 3        | 0.14          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 3        | 0.14          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 7        | 0.14          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 7        | 0.14          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 7        | 0.14          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 8        | 0.14          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 8        | 0.14          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 8        | 0.14          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 12       | 0.14          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 12       | 0.14          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 12       | 0.14          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 16       | 0.14          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 16       | 0.14          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 16       | 0.14          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 29       | 0.14          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 29       | 0.14          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 29       | 0.14          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 33       | 0.14          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 33       | 0.14          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 33       | 0.14          |
| (1,1559) | 1:10:A:ILE:HD11 | 1:10:A:ILE:HA   | 36       | 0.14          |
| (1,1559) | 1:10:A:ILE:HD12 | 1:10:A:ILE:HA   | 36       | 0.14          |
| (1,1559) | 1:10:A:ILE:HD13 | 1:10:A:ILE:HA   | 36       | 0.14          |
| (1,1550) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA    | 29       | 0.14          |
| (1,1550) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA    | 29       | 0.14          |
| (1,1550) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA    | 29       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H    | 3        | 0.14          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H    | 3        | 0.14          |

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| Key      | Atom-1          | Atom-2       | Model ID | Violation (Å) |
|----------|-----------------|--------------|----------|---------------|
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 3        | 0.14          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 5        | 0.14          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 5        | 0.14          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 5        | 0.14          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 6        | 0.14          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 6        | 0.14          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 6        | 0.14          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 7        | 0.14          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 7        | 0.14          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 7        | 0.14          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 9        | 0.14          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 9        | 0.14          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 9        | 0.14          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 10       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 10       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 10       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 12       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 12       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 12       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 16       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 16       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 16       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 17       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 17       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 17       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 18       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 18       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 18       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 19       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 19       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 19       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 20       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 20       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 20       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 23       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 23       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 23       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 25       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 25       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 25       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 26       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 26       | 0.14          |

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| Key      | Atom-1          | Atom-2       | Model ID | Violation (Å) |
|----------|-----------------|--------------|----------|---------------|
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 26       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 29       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 29       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 29       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 30       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 30       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 30       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 31       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 31       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 31       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 32       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 32       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 32       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 33       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 33       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 33       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 34       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 34       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 34       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 37       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 37       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 37       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 38       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 38       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 38       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H | 39       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H | 39       | 0.14          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H | 39       | 0.14          |
| (1,1535) | 1:2:A:ILE:HD11  | 1:2:A:ILE:HA | 29       | 0.14          |
| (1,1535) | 1:2:A:ILE:HD12  | 1:2:A:ILE:HA | 29       | 0.14          |
| (1,1535) | 1:2:A:ILE:HD13  | 1:2:A:ILE:HA | 29       | 0.14          |
| (1,1514) | 1:66:A:MET:HE1  | 1:66:A:MET:H | 2        | 0.14          |
| (1,1514) | 1:66:A:MET:HE2  | 1:66:A:MET:H | 2        | 0.14          |
| (1,1514) | 1:66:A:MET:HE3  | 1:66:A:MET:H | 2        | 0.14          |
| (1,1514) | 1:66:A:MET:HE1  | 1:66:A:MET:H | 7        | 0.14          |
| (1,1514) | 1:66:A:MET:HE2  | 1:66:A:MET:H | 7        | 0.14          |
| (1,1514) | 1:66:A:MET:HE3  | 1:66:A:MET:H | 7        | 0.14          |
| (1,1514) | 1:66:A:MET:HE1  | 1:66:A:MET:H | 11       | 0.14          |
| (1,1514) | 1:66:A:MET:HE2  | 1:66:A:MET:H | 11       | 0.14          |
| (1,1514) | 1:66:A:MET:HE3  | 1:66:A:MET:H | 11       | 0.14          |
| (1,1514) | 1:66:A:MET:HE1  | 1:66:A:MET:H | 18       | 0.14          |
| (1,1514) | 1:66:A:MET:HE2  | 1:66:A:MET:H | 18       | 0.14          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1514) | 1:66:A:MET:HE3 | 1:66:A:MET:H   | 18       | 0.14          |
| (1,1514) | 1:66:A:MET:HE1 | 1:66:A:MET:H   | 23       | 0.14          |
| (1,1514) | 1:66:A:MET:HE2 | 1:66:A:MET:H   | 23       | 0.14          |
| (1,1514) | 1:66:A:MET:HE3 | 1:66:A:MET:H   | 23       | 0.14          |
| (1,1514) | 1:66:A:MET:HE1 | 1:66:A:MET:H   | 25       | 0.14          |
| (1,1514) | 1:66:A:MET:HE2 | 1:66:A:MET:H   | 25       | 0.14          |
| (1,1514) | 1:66:A:MET:HE3 | 1:66:A:MET:H   | 25       | 0.14          |
| (1,1514) | 1:66:A:MET:HE1 | 1:66:A:MET:H   | 30       | 0.14          |
| (1,1514) | 1:66:A:MET:HE2 | 1:66:A:MET:H   | 30       | 0.14          |
| (1,1514) | 1:66:A:MET:HE3 | 1:66:A:MET:H   | 30       | 0.14          |
| (1,1514) | 1:66:A:MET:HE1 | 1:66:A:MET:H   | 31       | 0.14          |
| (1,1514) | 1:66:A:MET:HE2 | 1:66:A:MET:H   | 31       | 0.14          |
| (1,1514) | 1:66:A:MET:HE3 | 1:66:A:MET:H   | 31       | 0.14          |
| (1,1514) | 1:66:A:MET:HE1 | 1:66:A:MET:H   | 33       | 0.14          |
| (1,1514) | 1:66:A:MET:HE2 | 1:66:A:MET:H   | 33       | 0.14          |
| (1,1514) | 1:66:A:MET:HE3 | 1:66:A:MET:H   | 33       | 0.14          |
| (1,1514) | 1:66:A:MET:HE1 | 1:66:A:MET:H   | 39       | 0.14          |
| (1,1514) | 1:66:A:MET:HE2 | 1:66:A:MET:H   | 39       | 0.14          |
| (1,1514) | 1:66:A:MET:HE3 | 1:66:A:MET:H   | 39       | 0.14          |
| (1,1513) | 1:66:A:MET:HE1 | 1:29:A:PHE:H   | 1        | 0.14          |
| (1,1513) | 1:66:A:MET:HE2 | 1:29:A:PHE:H   | 1        | 0.14          |
| (1,1513) | 1:66:A:MET:HE3 | 1:29:A:PHE:H   | 1        | 0.14          |
| (1,1513) | 1:66:A:MET:HE1 | 1:29:A:PHE:H   | 5        | 0.14          |
| (1,1513) | 1:66:A:MET:HE2 | 1:29:A:PHE:H   | 5        | 0.14          |
| (1,1513) | 1:66:A:MET:HE3 | 1:29:A:PHE:H   | 5        | 0.14          |
| (1,1513) | 1:66:A:MET:HE1 | 1:29:A:PHE:H   | 23       | 0.14          |
| (1,1513) | 1:66:A:MET:HE2 | 1:29:A:PHE:H   | 23       | 0.14          |
| (1,1513) | 1:66:A:MET:HE3 | 1:29:A:PHE:H   | 23       | 0.14          |
| (1,1513) | 1:66:A:MET:HE1 | 1:29:A:PHE:H   | 37       | 0.14          |
| (1,1513) | 1:66:A:MET:HE2 | 1:29:A:PHE:H   | 37       | 0.14          |
| (1,1513) | 1:66:A:MET:HE3 | 1:29:A:PHE:H   | 37       | 0.14          |
| (1,1510) | 1:66:A:MET:HE1 | 1:42:A:TRP:HE1 | 16       | 0.14          |
| (1,1510) | 1:66:A:MET:HE2 | 1:42:A:TRP:HE1 | 16       | 0.14          |
| (1,1510) | 1:66:A:MET:HE3 | 1:42:A:TRP:HE1 | 16       | 0.14          |
| (1,1510) | 1:66:A:MET:HE1 | 1:42:A:TRP:HE1 | 28       | 0.14          |
| (1,1510) | 1:66:A:MET:HE2 | 1:42:A:TRP:HE1 | 28       | 0.14          |
| (1,1510) | 1:66:A:MET:HE3 | 1:42:A:TRP:HE1 | 28       | 0.14          |
| (1,1510) | 1:66:A:MET:HE1 | 1:42:A:TRP:HE1 | 33       | 0.14          |
| (1,1510) | 1:66:A:MET:HE2 | 1:42:A:TRP:HE1 | 33       | 0.14          |
| (1,1510) | 1:66:A:MET:HE3 | 1:42:A:TRP:HE1 | 33       | 0.14          |
| (1,1510) | 1:66:A:MET:HE1 | 1:42:A:TRP:HE1 | 39       | 0.14          |
| (1,1510) | 1:66:A:MET:HE2 | 1:42:A:TRP:HE1 | 39       | 0.14          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1510) | 1:66:A:MET:HE3 | 1:42:A:TRP:HE1 | 39       | 0.14          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 4        | 0.14          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 4        | 0.14          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 4        | 0.14          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 4        | 0.14          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 4        | 0.14          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 4        | 0.14          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 7        | 0.14          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 7        | 0.14          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 7        | 0.14          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 7        | 0.14          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 7        | 0.14          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 7        | 0.14          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 12       | 0.14          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 12       | 0.14          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 12       | 0.14          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 12       | 0.14          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 12       | 0.14          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 12       | 0.14          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 21       | 0.14          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 21       | 0.14          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 21       | 0.14          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 21       | 0.14          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 21       | 0.14          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 21       | 0.14          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 23       | 0.14          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 23       | 0.14          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 23       | 0.14          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 23       | 0.14          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 23       | 0.14          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 23       | 0.14          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 40       | 0.14          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 40       | 0.14          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 40       | 0.14          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 40       | 0.14          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 40       | 0.14          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 40       | 0.14          |
| (1,1508) | 1:66:A:MET:HE1 | 1:42:A:TRP:HZ3 | 8        | 0.14          |
| (1,1508) | 1:66:A:MET:HE2 | 1:42:A:TRP:HZ3 | 8        | 0.14          |
| (1,1508) | 1:66:A:MET:HE3 | 1:42:A:TRP:HZ3 | 8        | 0.14          |
| (1,1508) | 1:66:A:MET:HE1 | 1:42:A:TRP:HZ3 | 13       | 0.14          |
| (1,1508) | 1:66:A:MET:HE2 | 1:42:A:TRP:HZ3 | 13       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1508) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3  | 13       | 0.14          |
| (1,1508) | 1:66:A:MET:HE1  | 1:42:A:TRP:HZ3  | 18       | 0.14          |
| (1,1508) | 1:66:A:MET:HE2  | 1:42:A:TRP:HZ3  | 18       | 0.14          |
| (1,1508) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3  | 18       | 0.14          |
| (1,1508) | 1:66:A:MET:HE1  | 1:42:A:TRP:HZ3  | 35       | 0.14          |
| (1,1508) | 1:66:A:MET:HE2  | 1:42:A:TRP:HZ3  | 35       | 0.14          |
| (1,1508) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3  | 35       | 0.14          |
| (1,1507) | 1:66:A:MET:HE1  | 1:42:A:TRP:HB2  | 27       | 0.14          |
| (1,1507) | 1:66:A:MET:HE2  | 1:42:A:TRP:HB2  | 27       | 0.14          |
| (1,1507) | 1:66:A:MET:HE3  | 1:42:A:TRP:HB2  | 27       | 0.14          |
| (1,1502) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD11 | 27       | 0.14          |
| (1,1502) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD12 | 27       | 0.14          |
| (1,1502) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD13 | 27       | 0.14          |
| (1,1502) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD11 | 27       | 0.14          |
| (1,1502) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD12 | 27       | 0.14          |
| (1,1502) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD13 | 27       | 0.14          |
| (1,1502) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD11 | 27       | 0.14          |
| (1,1502) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD12 | 27       | 0.14          |
| (1,1502) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD13 | 27       | 0.14          |
| (1,1500) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2  | 4        | 0.14          |
| (1,1500) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2  | 4        | 0.14          |
| (1,1500) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2  | 4        | 0.14          |
| (1,1500) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2  | 15       | 0.14          |
| (1,1500) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2  | 15       | 0.14          |
| (1,1500) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2  | 15       | 0.14          |
| (1,1500) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2  | 16       | 0.14          |
| (1,1500) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2  | 16       | 0.14          |
| (1,1500) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2  | 16       | 0.14          |
| (1,1500) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2  | 29       | 0.14          |
| (1,1500) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2  | 29       | 0.14          |
| (1,1500) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2  | 29       | 0.14          |
| (1,1500) | 1:66:A:MET:HE1  | 1:66:A:MET:HB2  | 39       | 0.14          |
| (1,1500) | 1:66:A:MET:HE2  | 1:66:A:MET:HB2  | 39       | 0.14          |
| (1,1500) | 1:66:A:MET:HE3  | 1:66:A:MET:HB2  | 39       | 0.14          |
| (1,1494) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 9        | 0.14          |
| (1,1494) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 9        | 0.14          |
| (1,1494) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 9        | 0.14          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA   | 7        | 0.14          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA   | 7        | 0.14          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA   | 7        | 0.14          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA   | 31       | 0.14          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA   | 31       | 0.14          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA  | 31       | 0.14          |
| (1,1484) | 1:81:A:VAL:HB   | 1:42:A:TRP:HE1 | 5        | 0.14          |
| (1,1484) | 1:81:A:VAL:HB   | 1:42:A:TRP:HE1 | 14       | 0.14          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H   | 1        | 0.14          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H   | 1        | 0.14          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H   | 1        | 0.14          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H   | 2        | 0.14          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H   | 2        | 0.14          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H   | 2        | 0.14          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H   | 4        | 0.14          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H   | 4        | 0.14          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H   | 4        | 0.14          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H   | 9        | 0.14          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H   | 9        | 0.14          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H   | 9        | 0.14          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H   | 10       | 0.14          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H   | 10       | 0.14          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H   | 10       | 0.14          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H   | 15       | 0.14          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H   | 15       | 0.14          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H   | 15       | 0.14          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H   | 18       | 0.14          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H   | 18       | 0.14          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H   | 18       | 0.14          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H   | 22       | 0.14          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H   | 22       | 0.14          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H   | 22       | 0.14          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H   | 26       | 0.14          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H   | 26       | 0.14          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H   | 26       | 0.14          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H   | 27       | 0.14          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H   | 27       | 0.14          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H   | 27       | 0.14          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H   | 31       | 0.14          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H   | 31       | 0.14          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H   | 31       | 0.14          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H   | 32       | 0.14          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H   | 32       | 0.14          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H   | 32       | 0.14          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H   | 35       | 0.14          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H   | 35       | 0.14          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H   | 35       | 0.14          |

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| Key      | Atom-1          | Atom-2       | Model ID | Violation (Å) |
|----------|-----------------|--------------|----------|---------------|
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 39       | 0.14          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 39       | 0.14          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 39       | 0.14          |
| (1,1463) | 1:71:A:VAL:HG21 | 1:72:A:THR:H | 18       | 0.14          |
| (1,1463) | 1:71:A:VAL:HG22 | 1:72:A:THR:H | 18       | 0.14          |
| (1,1463) | 1:71:A:VAL:HG23 | 1:72:A:THR:H | 18       | 0.14          |
| (1,1403) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H | 1        | 0.14          |
| (1,1403) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H | 1        | 0.14          |
| (1,1403) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H | 1        | 0.14          |
| (1,1403) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H | 4        | 0.14          |
| (1,1403) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H | 4        | 0.14          |
| (1,1403) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H | 4        | 0.14          |
| (1,1403) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H | 10       | 0.14          |
| (1,1403) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H | 10       | 0.14          |
| (1,1403) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H | 10       | 0.14          |
| (1,1403) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H | 16       | 0.14          |
| (1,1403) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H | 16       | 0.14          |
| (1,1403) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H | 16       | 0.14          |
| (1,1403) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H | 27       | 0.14          |
| (1,1403) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H | 27       | 0.14          |
| (1,1403) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H | 27       | 0.14          |
| (1,1403) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H | 29       | 0.14          |
| (1,1403) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H | 29       | 0.14          |
| (1,1403) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H | 29       | 0.14          |
| (1,1403) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H | 34       | 0.14          |
| (1,1403) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H | 34       | 0.14          |
| (1,1403) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H | 34       | 0.14          |
| (1,1403) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H | 39       | 0.14          |
| (1,1403) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H | 39       | 0.14          |
| (1,1403) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H | 39       | 0.14          |
| (1,1401) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H | 9        | 0.14          |
| (1,1401) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H | 9        | 0.14          |
| (1,1401) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H | 9        | 0.14          |
| (1,1401) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H | 36       | 0.14          |
| (1,1401) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H | 36       | 0.14          |
| (1,1401) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H | 36       | 0.14          |
| (1,1401) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H | 38       | 0.14          |
| (1,1401) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H | 38       | 0.14          |
| (1,1401) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H | 38       | 0.14          |
| (1,1401) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H | 39       | 0.14          |
| (1,1401) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H | 39       | 0.14          |
| (1,1401) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H | 39       | 0.14          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 2        | 0.14          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 2        | 0.14          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 2        | 0.14          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 3        | 0.14          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 3        | 0.14          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 3        | 0.14          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 4        | 0.14          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 4        | 0.14          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 4        | 0.14          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 5        | 0.14          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 5        | 0.14          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 5        | 0.14          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 6        | 0.14          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 6        | 0.14          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 6        | 0.14          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 14       | 0.14          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 14       | 0.14          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 14       | 0.14          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 16       | 0.14          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 16       | 0.14          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 16       | 0.14          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 22       | 0.14          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 22       | 0.14          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 22       | 0.14          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 25       | 0.14          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 25       | 0.14          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 25       | 0.14          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 27       | 0.14          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 27       | 0.14          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 27       | 0.14          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 31       | 0.14          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 31       | 0.14          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 31       | 0.14          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 32       | 0.14          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 32       | 0.14          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 32       | 0.14          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 39       | 0.14          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 39       | 0.14          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 39       | 0.14          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 40       | 0.14          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 40       | 0.14          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 40       | 0.14          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1387) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ  | 3        | 0.14          |
| (1,1387) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ  | 3        | 0.14          |
| (1,1387) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ  | 3        | 0.14          |
| (1,1387) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ  | 5        | 0.14          |
| (1,1387) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ  | 5        | 0.14          |
| (1,1387) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ  | 5        | 0.14          |
| (1,1387) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ  | 10       | 0.14          |
| (1,1387) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ  | 10       | 0.14          |
| (1,1387) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ  | 10       | 0.14          |
| (1,1387) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ  | 35       | 0.14          |
| (1,1387) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ  | 35       | 0.14          |
| (1,1387) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ  | 35       | 0.14          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 24       | 0.14          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 24       | 0.14          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 24       | 0.14          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 24       | 0.14          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 24       | 0.14          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 24       | 0.14          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 24       | 0.14          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 24       | 0.14          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 24       | 0.14          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 40       | 0.14          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 40       | 0.14          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 40       | 0.14          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 40       | 0.14          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 40       | 0.14          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 40       | 0.14          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 40       | 0.14          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 40       | 0.14          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 40       | 0.14          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 24       | 0.14          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 24       | 0.14          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 24       | 0.14          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 24       | 0.14          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 24       | 0.14          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 24       | 0.14          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 24       | 0.14          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 24       | 0.14          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 24       | 0.14          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 40       | 0.14          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 40       | 0.14          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 40       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1379) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB1  | 40       | 0.14          |
| (1,1379) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB2  | 40       | 0.14          |
| (1,1379) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB3  | 40       | 0.14          |
| (1,1379) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB1  | 40       | 0.14          |
| (1,1379) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB2  | 40       | 0.14          |
| (1,1379) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB3  | 40       | 0.14          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 6        | 0.14          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 16       | 0.14          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 33       | 0.14          |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H    | 8        | 0.14          |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H    | 8        | 0.14          |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H    | 8        | 0.14          |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H    | 16       | 0.14          |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H    | 16       | 0.14          |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H    | 16       | 0.14          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 4        | 0.14          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 10       | 0.14          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 11       | 0.14          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 14       | 0.14          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 15       | 0.14          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 19       | 0.14          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 20       | 0.14          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 23       | 0.14          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 25       | 0.14          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 26       | 0.14          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 29       | 0.14          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 30       | 0.14          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 31       | 0.14          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 32       | 0.14          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 33       | 0.14          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 35       | 0.14          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 36       | 0.14          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 37       | 0.14          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 39       | 0.14          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 40       | 0.14          |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 9        | 0.14          |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 15       | 0.14          |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 29       | 0.14          |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 35       | 0.14          |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 36       | 0.14          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 12       | 0.14          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 12       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 12       | 0.14          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 19       | 0.14          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 19       | 0.14          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 19       | 0.14          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 21       | 0.14          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 21       | 0.14          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 21       | 0.14          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 31       | 0.14          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 31       | 0.14          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 31       | 0.14          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1  | 17       | 0.14          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2  | 17       | 0.14          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3  | 17       | 0.14          |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1  | 17       | 0.14          |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2  | 17       | 0.14          |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3  | 17       | 0.14          |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1  | 17       | 0.14          |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2  | 17       | 0.14          |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3  | 17       | 0.14          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1  | 20       | 0.14          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2  | 20       | 0.14          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3  | 20       | 0.14          |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1  | 20       | 0.14          |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2  | 20       | 0.14          |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3  | 20       | 0.14          |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1  | 20       | 0.14          |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2  | 20       | 0.14          |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3  | 20       | 0.14          |
| (1,1289) | 1:40:A:VAL:HG21 | 1:42:A:TRP:HE1  | 35       | 0.14          |
| (1,1289) | 1:40:A:VAL:HG22 | 1:42:A:TRP:HE1  | 35       | 0.14          |
| (1,1289) | 1:40:A:VAL:HG23 | 1:42:A:TRP:HE1  | 35       | 0.14          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 12       | 0.14          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 12       | 0.14          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 12       | 0.14          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 19       | 0.14          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 19       | 0.14          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 19       | 0.14          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 21       | 0.14          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 21       | 0.14          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 21       | 0.14          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 31       | 0.14          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 31       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 31       | 0.14          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 1        | 0.14          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 1        | 0.14          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 1        | 0.14          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 1        | 0.14          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 1        | 0.14          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 1        | 0.14          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 1        | 0.14          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 1        | 0.14          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 1        | 0.14          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 4        | 0.14          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 4        | 0.14          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 4        | 0.14          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 4        | 0.14          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 4        | 0.14          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 4        | 0.14          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 4        | 0.14          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 4        | 0.14          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 4        | 0.14          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 17       | 0.14          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 17       | 0.14          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 17       | 0.14          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 17       | 0.14          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 17       | 0.14          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 17       | 0.14          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 17       | 0.14          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 17       | 0.14          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 17       | 0.14          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 18       | 0.14          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 18       | 0.14          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 18       | 0.14          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 18       | 0.14          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 18       | 0.14          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 18       | 0.14          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 18       | 0.14          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 18       | 0.14          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 18       | 0.14          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 22       | 0.14          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 22       | 0.14          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 22       | 0.14          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 22       | 0.14          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 22       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 22       | 0.14          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 22       | 0.14          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 22       | 0.14          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 22       | 0.14          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 30       | 0.14          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 30       | 0.14          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 30       | 0.14          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 30       | 0.14          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 30       | 0.14          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 30       | 0.14          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 30       | 0.14          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 30       | 0.14          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 30       | 0.14          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 34       | 0.14          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 34       | 0.14          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 34       | 0.14          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 34       | 0.14          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 34       | 0.14          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 34       | 0.14          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 34       | 0.14          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 34       | 0.14          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 34       | 0.14          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 10       | 0.14          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 10       | 0.14          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 10       | 0.14          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 11       | 0.14          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 11       | 0.14          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 11       | 0.14          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 13       | 0.14          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 13       | 0.14          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 13       | 0.14          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 33       | 0.14          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 33       | 0.14          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 33       | 0.14          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 34       | 0.14          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 34       | 0.14          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 34       | 0.14          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 35       | 0.14          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 35       | 0.14          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 35       | 0.14          |
| (1,1263) | 1:94:A:THR:HG21 | 1:94:A:THR:HA   | 28       | 0.14          |
| (1,1263) | 1:94:A:THR:HG22 | 1:94:A:THR:HA   | 28       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1263) | 1:94:A:THR:HG23 | 1:94:A:THR:HA   | 28       | 0.14          |
| (1,1261) | 1:67:A:THR:HG21 | 1:56:A:ASN:H    | 23       | 0.14          |
| (1,1261) | 1:67:A:THR:HG22 | 1:56:A:ASN:H    | 23       | 0.14          |
| (1,1261) | 1:67:A:THR:HG23 | 1:56:A:ASN:H    | 23       | 0.14          |
| (1,1257) | 1:67:A:THR:HG21 | 1:26:A:SER:HB2  | 4        | 0.14          |
| (1,1257) | 1:67:A:THR:HG22 | 1:26:A:SER:HB2  | 4        | 0.14          |
| (1,1257) | 1:67:A:THR:HG23 | 1:26:A:SER:HB2  | 4        | 0.14          |
| (1,1257) | 1:67:A:THR:HG21 | 1:26:A:SER:HB2  | 30       | 0.14          |
| (1,1257) | 1:67:A:THR:HG22 | 1:26:A:SER:HB2  | 30       | 0.14          |
| (1,1257) | 1:67:A:THR:HG23 | 1:26:A:SER:HB2  | 30       | 0.14          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 22       | 0.14          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 22       | 0.14          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 22       | 0.14          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 30       | 0.14          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 30       | 0.14          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 30       | 0.14          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3  | 31       | 0.14          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3  | 31       | 0.14          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3  | 31       | 0.14          |
| (1,1248) | 1:28:A:THR:HG21 | 1:67:A:THR:HG21 | 9        | 0.14          |
| (1,1248) | 1:28:A:THR:HG21 | 1:67:A:THR:HG22 | 9        | 0.14          |
| (1,1248) | 1:28:A:THR:HG21 | 1:67:A:THR:HG23 | 9        | 0.14          |
| (1,1248) | 1:28:A:THR:HG22 | 1:67:A:THR:HG21 | 9        | 0.14          |
| (1,1248) | 1:28:A:THR:HG22 | 1:67:A:THR:HG22 | 9        | 0.14          |
| (1,1248) | 1:28:A:THR:HG22 | 1:67:A:THR:HG23 | 9        | 0.14          |
| (1,1248) | 1:28:A:THR:HG23 | 1:67:A:THR:HG21 | 9        | 0.14          |
| (1,1248) | 1:28:A:THR:HG23 | 1:67:A:THR:HG22 | 9        | 0.14          |
| (1,1248) | 1:28:A:THR:HG23 | 1:67:A:THR:HG23 | 9        | 0.14          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 1        | 0.14          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 1        | 0.14          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 1        | 0.14          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 7        | 0.14          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 7        | 0.14          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 7        | 0.14          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 17       | 0.14          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 17       | 0.14          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 17       | 0.14          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 19       | 0.14          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 19       | 0.14          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 19       | 0.14          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 24       | 0.14          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 24       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 24       | 0.14          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 25       | 0.14          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 25       | 0.14          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 25       | 0.14          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 34       | 0.14          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 34       | 0.14          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 34       | 0.14          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 35       | 0.14          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 35       | 0.14          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 35       | 0.14          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 39       | 0.14          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 39       | 0.14          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 39       | 0.14          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 40       | 0.14          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 40       | 0.14          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 40       | 0.14          |
| (1,1239) | 1:13:A:THR:HG21 | 1:34:A:SER:H    | 21       | 0.14          |
| (1,1239) | 1:13:A:THR:HG22 | 1:34:A:SER:H    | 21       | 0.14          |
| (1,1239) | 1:13:A:THR:HG23 | 1:34:A:SER:H    | 21       | 0.14          |
| (1,1239) | 1:13:A:THR:HG21 | 1:34:A:SER:H    | 32       | 0.14          |
| (1,1239) | 1:13:A:THR:HG22 | 1:34:A:SER:H    | 32       | 0.14          |
| (1,1239) | 1:13:A:THR:HG23 | 1:34:A:SER:H    | 32       | 0.14          |
| (1,1236) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3  | 15       | 0.14          |
| (1,1236) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3  | 15       | 0.14          |
| (1,1236) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3  | 15       | 0.14          |
| (1,1236) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3  | 25       | 0.14          |
| (1,1236) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3  | 25       | 0.14          |
| (1,1236) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3  | 25       | 0.14          |
| (1,1226) | 1:101:A:LEU:H   | 1:22:A:SER:HA   | 6        | 0.14          |
| (1,1226) | 1:101:A:LEU:H   | 1:22:A:SER:HA   | 7        | 0.14          |
| (1,1226) | 1:101:A:LEU:H   | 1:22:A:SER:HA   | 19       | 0.14          |
| (1,1226) | 1:101:A:LEU:H   | 1:22:A:SER:HA   | 26       | 0.14          |
| (1,1226) | 1:101:A:LEU:H   | 1:22:A:SER:HA   | 39       | 0.14          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 20       | 0.14          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 20       | 0.14          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 20       | 0.14          |
| (1,1213) | 1:66:A:MET:H    | 1:28:A:THR:HA   | 4        | 0.14          |
| (1,1213) | 1:66:A:MET:H    | 1:28:A:THR:HA   | 7        | 0.14          |
| (1,1213) | 1:66:A:MET:H    | 1:28:A:THR:HA   | 31       | 0.14          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG21 | 24       | 0.14          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG22 | 24       | 0.14          |
| (1,1190) | 1:22:A:SER:H    | 1:21:A:VAL:HG23 | 24       | 0.14          |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1190) | 1:22:A:SER:H  | 1:21:A:VAL:HG21 | 33       | 0.14          |
| (1,1190) | 1:22:A:SER:H  | 1:21:A:VAL:HG22 | 33       | 0.14          |
| (1,1190) | 1:22:A:SER:H  | 1:21:A:VAL:HG23 | 33       | 0.14          |
| (1,1185) | 1:21:A:VAL:H  | 1:100:A:GLU:HB3 | 14       | 0.14          |
| (1,1177) | 1:100:A:GLU:H | 1:21:A:VAL:HG11 | 15       | 0.14          |
| (1,1177) | 1:100:A:GLU:H | 1:21:A:VAL:HG12 | 15       | 0.14          |
| (1,1177) | 1:100:A:GLU:H | 1:21:A:VAL:HG13 | 15       | 0.14          |
| (1,1174) | 1:91:A:ALA:H  | 1:84:A:ARG:HA   | 11       | 0.14          |
| (1,1174) | 1:91:A:ALA:H  | 1:84:A:ARG:HA   | 15       | 0.14          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 23       | 0.14          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 23       | 0.14          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 30       | 0.14          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 30       | 0.14          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE1  | 36       | 0.14          |
| (1,1162) | 1:97:A:LEU:H  | 1:29:A:PHE:HE2  | 36       | 0.14          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 30       | 0.14          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 32       | 0.14          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 35       | 0.14          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 37       | 0.14          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 38       | 0.14          |
| (1,1084) | 1:99:A:GLY:H  | 1:99:A:GLY:HA2  | 6        | 0.14          |
| (1,1084) | 1:99:A:GLY:H  | 1:99:A:GLY:HA2  | 7        | 0.14          |
| (1,1084) | 1:99:A:GLY:H  | 1:99:A:GLY:HA2  | 9        | 0.14          |
| (1,1084) | 1:99:A:GLY:H  | 1:99:A:GLY:HA2  | 15       | 0.14          |
| (1,1084) | 1:99:A:GLY:H  | 1:99:A:GLY:HA2  | 25       | 0.14          |
| (1,1084) | 1:99:A:GLY:H  | 1:99:A:GLY:HA2  | 27       | 0.14          |
| (1,1084) | 1:99:A:GLY:H  | 1:99:A:GLY:HA2  | 28       | 0.14          |
| (1,1084) | 1:99:A:GLY:H  | 1:99:A:GLY:HA2  | 30       | 0.14          |
| (1,1084) | 1:99:A:GLY:H  | 1:99:A:GLY:HA2  | 32       | 0.14          |
| (1,1084) | 1:99:A:GLY:H  | 1:99:A:GLY:HA2  | 34       | 0.14          |
| (1,1084) | 1:99:A:GLY:H  | 1:99:A:GLY:HA2  | 35       | 0.14          |
| (1,1084) | 1:99:A:GLY:H  | 1:99:A:GLY:HA2  | 36       | 0.14          |
| (1,1084) | 1:99:A:GLY:H  | 1:99:A:GLY:HA2  | 37       | 0.14          |
| (1,1084) | 1:99:A:GLY:H  | 1:99:A:GLY:HA2  | 38       | 0.14          |
| (1,1052) | 1:26:A:SER:H  | 1:25:A:GLN:HG2  | 10       | 0.14          |
| (1,1052) | 1:26:A:SER:H  | 1:25:A:GLN:HG2  | 16       | 0.14          |
| (1,1052) | 1:26:A:SER:H  | 1:25:A:GLN:HG2  | 18       | 0.14          |
| (1,1052) | 1:26:A:SER:H  | 1:25:A:GLN:HG2  | 26       | 0.14          |
| (1,1052) | 1:26:A:SER:H  | 1:25:A:GLN:HG2  | 28       | 0.14          |
| (1,1052) | 1:26:A:SER:H  | 1:25:A:GLN:HG2  | 31       | 0.14          |
| (1,1052) | 1:26:A:SER:H  | 1:25:A:GLN:HG2  | 34       | 0.14          |
| (1,1052) | 1:26:A:SER:H  | 1:25:A:GLN:HG2  | 35       | 0.14          |

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| Key      | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|----------|--------------|-----------------|----------|---------------|
| (1,1043) | 1:26:A:SER:H | 1:26:A:SER:HB3  | 14       | 0.14          |
| (1,1043) | 1:26:A:SER:H | 1:26:A:SER:HB3  | 26       | 0.14          |
| (1,1020) | 1:48:A:GLU:H | 1:48:A:GLU:HG3  | 9        | 0.14          |
| (1,1020) | 1:48:A:GLU:H | 1:48:A:GLU:HG3  | 17       | 0.14          |
| (1,1020) | 1:48:A:GLU:H | 1:48:A:GLU:HG3  | 18       | 0.14          |
| (1,1020) | 1:48:A:GLU:H | 1:48:A:GLU:HG3  | 35       | 0.14          |
| (1,1002) | 1:5:A:PHE:H  | 1:4:A:PRO:HA    | 29       | 0.14          |
| (1,987)  | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 5        | 0.14          |
| (1,987)  | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 21       | 0.14          |
| (1,987)  | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 23       | 0.14          |
| (1,987)  | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 27       | 0.14          |
| (1,987)  | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 31       | 0.14          |
| (1,987)  | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 39       | 0.14          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 4        | 0.14          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 10       | 0.14          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 11       | 0.14          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 14       | 0.14          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 15       | 0.14          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 19       | 0.14          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 20       | 0.14          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 23       | 0.14          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 25       | 0.14          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 26       | 0.14          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 29       | 0.14          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 30       | 0.14          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 31       | 0.14          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 32       | 0.14          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 33       | 0.14          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 35       | 0.14          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 36       | 0.14          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 37       | 0.14          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 39       | 0.14          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 40       | 0.14          |
| (1,971)  | 1:21:A:VAL:H | 1:21:A:VAL:HG21 | 6        | 0.14          |
| (1,971)  | 1:21:A:VAL:H | 1:21:A:VAL:HG22 | 6        | 0.14          |
| (1,971)  | 1:21:A:VAL:H | 1:21:A:VAL:HG23 | 6        | 0.14          |
| (1,967)  | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 1        | 0.14          |
| (1,967)  | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 13       | 0.14          |
| (1,967)  | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 23       | 0.14          |
| (1,967)  | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 26       | 0.14          |
| (1,941)  | 1:34:A:SER:H | 1:12:A:PHE:HA   | 8        | 0.14          |
| (1,941)  | 1:34:A:SER:H | 1:12:A:PHE:HA   | 16       | 0.14          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,941) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 21       | 0.14          |
| (1,941) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 22       | 0.14          |
| (1,941) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 27       | 0.14          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 5        | 0.14          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 5        | 0.14          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 5        | 0.14          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 14       | 0.14          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 14       | 0.14          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 14       | 0.14          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 17       | 0.14          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 17       | 0.14          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 17       | 0.14          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 18       | 0.14          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 18       | 0.14          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 18       | 0.14          |
| (1,932) | 1:98:A:LYS:H | 1:19:A:ILE:HB   | 19       | 0.14          |
| (1,932) | 1:98:A:LYS:H | 1:19:A:ILE:HB   | 30       | 0.14          |
| (1,918) | 1:37:A:ASP:H | 1:36:A:ASP:HB3  | 36       | 0.14          |
| (1,915) | 1:37:A:ASP:H | 1:37:A:ASP:HA   | 1        | 0.14          |
| (1,899) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 4        | 0.14          |
| (1,888) | 1:80:A:SER:H | 1:43:A:TYR:HB3  | 4        | 0.14          |
| (1,888) | 1:80:A:SER:H | 1:43:A:TYR:HB3  | 11       | 0.14          |
| (1,888) | 1:80:A:SER:H | 1:43:A:TYR:HB3  | 32       | 0.14          |
| (1,870) | 1:8:A:GLU:H  | 1:9:A:PRO:HD2   | 21       | 0.14          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 14       | 0.14          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 14       | 0.14          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 14       | 0.14          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 15       | 0.14          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 15       | 0.14          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 15       | 0.14          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 17       | 0.14          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 17       | 0.14          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 17       | 0.14          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 31       | 0.14          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 31       | 0.14          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 31       | 0.14          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 40       | 0.14          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 40       | 0.14          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 40       | 0.14          |
| (1,827) | 1:17:A:GLN:H | 1:17:A:GLN:HB2  | 8        | 0.14          |
| (1,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB   | 11       | 0.14          |
| (1,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB   | 14       | 0.14          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 1        | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 1        | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 1        | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 2        | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 2        | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 2        | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 4        | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 4        | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 4        | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 9        | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 9        | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 9        | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 10       | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 10       | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 10       | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 15       | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 15       | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 15       | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 18       | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 18       | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 18       | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 22       | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 22       | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 22       | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 26       | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 26       | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 26       | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 27       | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 27       | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 27       | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 31       | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 31       | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 31       | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 32       | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 32       | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 32       | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 35       | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 35       | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 35       | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 39       | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 39       | 0.14          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 39       | 0.14          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 26       | 0.14          |
| (1,717) | 1:16:A:ILE:H  | 1:15:A:ARG:HB2  | 19       | 0.14          |
| (1,683) | 1:23:A:GLU:H  | 1:22:A:SER:HB3  | 6        | 0.14          |
| (1,661) | 1:7:A:ALA:H   | 1:6:A:THR:HA    | 2        | 0.14          |
| (1,661) | 1:7:A:ALA:H   | 1:6:A:THR:HA    | 6        | 0.14          |
| (1,661) | 1:7:A:ALA:H   | 1:6:A:THR:HA    | 25       | 0.14          |
| (1,661) | 1:7:A:ALA:H   | 1:6:A:THR:HA    | 27       | 0.14          |
| (1,661) | 1:7:A:ALA:H   | 1:6:A:THR:HA    | 33       | 0.14          |
| (1,661) | 1:7:A:ALA:H   | 1:6:A:THR:HA    | 37       | 0.14          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 7        | 0.14          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 15       | 0.14          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 33       | 0.14          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 40       | 0.14          |
| (1,591) | 1:3:A:ASP:H   | 1:3:A:ASP:HA    | 9        | 0.14          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 5        | 0.14          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 5        | 0.14          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 5        | 0.14          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 8        | 0.14          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 8        | 0.14          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 8        | 0.14          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 24       | 0.14          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 24       | 0.14          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 24       | 0.14          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 31       | 0.14          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 31       | 0.14          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 31       | 0.14          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 40       | 0.14          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 40       | 0.14          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 40       | 0.14          |
| (1,560) | 1:47:A:THR:H  | 1:47:A:THR:HA   | 2        | 0.14          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 5        | 0.14          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2  | 5        | 0.14          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 13       | 0.14          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2  | 13       | 0.14          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 23       | 0.14          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2  | 23       | 0.14          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 25       | 0.14          |
| (1,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD2  | 25       | 0.14          |
| (1,549) | 1:71:A:VAL:H  | 1:70:A:ASN:HB2  | 10       | 0.14          |
| (1,531) | 1:99:A:GLY:H  | 1:98:A:LYS:HG2  | 7        | 0.14          |
| (1,531) | 1:99:A:GLY:H  | 1:98:A:LYS:HG2  | 11       | 0.14          |
| (1,531) | 1:99:A:GLY:H  | 1:98:A:LYS:HG2  | 19       | 0.14          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 34       | 0.14          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 10       | 0.14          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 12       | 0.14          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 16       | 0.14          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 24       | 0.14          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 25       | 0.14          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 26       | 0.14          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 27       | 0.14          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 30       | 0.14          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 32       | 0.14          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 40       | 0.14          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 16       | 0.14          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 24       | 0.14          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 26       | 0.14          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 32       | 0.14          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 40       | 0.14          |
| (1,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 10       | 0.14          |
| (1,419) | 1:69:A:HIS:H | 1:54:A:LYS:HA   | 12       | 0.14          |
| (1,410) | 1:96:A:GLU:H | 1:18:A:ASN:HD21 | 21       | 0.14          |
| (1,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD21 | 34       | 0.14          |
| (1,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD22 | 34       | 0.14          |
| (1,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD23 | 34       | 0.14          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 3        | 0.14          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 4        | 0.14          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 6        | 0.14          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 7        | 0.14          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 12       | 0.14          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 16       | 0.14          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 19       | 0.14          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 37       | 0.14          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 1        | 0.14          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 3        | 0.14          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 7        | 0.14          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 9        | 0.14          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 26       | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 1        | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 1        | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 1        | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 7        | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 7        | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 7        | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 17       | 0.14          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 17       | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 17       | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 18       | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 18       | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 18       | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 19       | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 19       | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 19       | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 21       | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 21       | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 21       | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 24       | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 24       | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 24       | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 33       | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 33       | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 33       | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 34       | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 34       | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 34       | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 35       | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 35       | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 35       | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 40       | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 40       | 0.14          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 40       | 0.14          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 1        | 0.14          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 1        | 0.14          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 1        | 0.14          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 4        | 0.14          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 4        | 0.14          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 4        | 0.14          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 10       | 0.14          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 10       | 0.14          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 10       | 0.14          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 16       | 0.14          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 16       | 0.14          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 16       | 0.14          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 27       | 0.14          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 27       | 0.14          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 27       | 0.14          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 29       | 0.14          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 29       | 0.14          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 29       | 0.14          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 34       | 0.14          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 34       | 0.14          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 34       | 0.14          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 39       | 0.14          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 39       | 0.14          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 39       | 0.14          |
| (1,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 1        | 0.14          |
| (1,368) | 1:18:A:ASN:H | 1:17:A:GLN:HB3  | 26       | 0.14          |
| (1,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD1  | 9        | 0.14          |
| (1,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD2  | 9        | 0.14          |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 5        | 0.14          |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 6        | 0.14          |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 7        | 0.14          |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 14       | 0.14          |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 16       | 0.14          |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 27       | 0.14          |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 28       | 0.14          |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 35       | 0.14          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 16       | 0.14          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1  | 1        | 0.14          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2  | 1        | 0.14          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1  | 18       | 0.14          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2  | 18       | 0.14          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1  | 34       | 0.14          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2  | 34       | 0.14          |
| (1,201) | 1:90:A:GLU:H | 1:89:A:GLY:HA2  | 6        | 0.14          |
| (1,201) | 1:90:A:GLU:H | 1:89:A:GLY:HA2  | 9        | 0.14          |
| (1,201) | 1:90:A:GLU:H | 1:89:A:GLY:HA2  | 28       | 0.14          |
| (1,199) | 1:90:A:GLU:H | 1:10:A:ILE:HG21 | 38       | 0.14          |
| (1,199) | 1:90:A:GLU:H | 1:10:A:ILE:HG22 | 38       | 0.14          |
| (1,199) | 1:90:A:GLU:H | 1:10:A:ILE:HG23 | 38       | 0.14          |
| (1,199) | 1:90:A:GLU:H | 1:10:A:ILE:HG21 | 40       | 0.14          |
| (1,199) | 1:90:A:GLU:H | 1:10:A:ILE:HG22 | 40       | 0.14          |
| (1,199) | 1:90:A:GLU:H | 1:10:A:ILE:HG23 | 40       | 0.14          |
| (1,198) | 1:90:A:GLU:H | 1:90:A:GLU:HB2  | 38       | 0.14          |
| (1,198) | 1:90:A:GLU:H | 1:90:A:GLU:HB2  | 39       | 0.14          |
| (1,148) | 1:45:A:GLY:H | 1:46:A:PRO:HD2  | 23       | 0.14          |
| (1,148) | 1:45:A:GLY:H | 1:46:A:PRO:HD2  | 25       | 0.14          |
| (1,148) | 1:45:A:GLY:H | 1:46:A:PRO:HD2  | 40       | 0.14          |
| (1,136) | 1:39:A:ILE:H | 1:10:A:ILE:HD11 | 11       | 0.14          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,136)  | 1:39:A:ILE:H   | 1:10:A:ILE:HD12 | 11       | 0.14          |
| (1,136)  | 1:39:A:ILE:H   | 1:10:A:ILE:HD13 | 11       | 0.14          |
| (1,136)  | 1:39:A:ILE:H   | 1:10:A:ILE:HD11 | 36       | 0.14          |
| (1,136)  | 1:39:A:ILE:H   | 1:10:A:ILE:HD12 | 36       | 0.14          |
| (1,136)  | 1:39:A:ILE:H   | 1:10:A:ILE:HD13 | 36       | 0.14          |
| (1,57)   | 1:42:A:TRP:H   | 1:41:A:THR:HB   | 7        | 0.14          |
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 2        | 0.14          |
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 3        | 0.14          |
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 5        | 0.14          |
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 8        | 0.14          |
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 10       | 0.14          |
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 11       | 0.14          |
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 12       | 0.14          |
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 14       | 0.14          |
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 16       | 0.14          |
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 20       | 0.14          |
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 21       | 0.14          |
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 24       | 0.14          |
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 25       | 0.14          |
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 26       | 0.14          |
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 27       | 0.14          |
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 29       | 0.14          |
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 31       | 0.14          |
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 32       | 0.14          |
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 33       | 0.14          |
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 37       | 0.14          |
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 40       | 0.14          |
| (1,37)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3  | 21       | 0.14          |
| (1,37)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3  | 31       | 0.14          |
| (1,37)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3  | 40       | 0.14          |
| (1,35)   | 1:88:A:ARG:H   | 1:88:A:ARG:HG2  | 1        | 0.14          |
| (1,35)   | 1:88:A:ARG:H   | 1:88:A:ARG:HG2  | 3        | 0.14          |
| (1,35)   | 1:88:A:ARG:H   | 1:88:A:ARG:HG2  | 5        | 0.14          |
| (1,35)   | 1:88:A:ARG:H   | 1:88:A:ARG:HG2  | 8        | 0.14          |
| (1,35)   | 1:88:A:ARG:H   | 1:88:A:ARG:HG2  | 11       | 0.14          |
| (1,35)   | 1:88:A:ARG:H   | 1:88:A:ARG:HG2  | 14       | 0.14          |
| (1,35)   | 1:88:A:ARG:H   | 1:88:A:ARG:HG2  | 16       | 0.14          |
| (3,3217) | 1:69:A:HIS:HE1 | 1:67:A:THR:HB   | 14       | 0.13          |
| (3,3217) | 1:69:A:HIS:HE1 | 1:67:A:THR:HB   | 21       | 0.13          |
| (3,3217) | 1:69:A:HIS:HE1 | 1:67:A:THR:HB   | 29       | 0.13          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 2        | 0.13          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 2        | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 12       | 0.13          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 12       | 0.13          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 21       | 0.13          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 21       | 0.13          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 32       | 0.13          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 32       | 0.13          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 33       | 0.13          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 33       | 0.13          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 8        | 0.13          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 8        | 0.13          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 8        | 0.13          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 8        | 0.13          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 8        | 0.13          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 8        | 0.13          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 13       | 0.13          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 13       | 0.13          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 13       | 0.13          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 13       | 0.13          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 13       | 0.13          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 13       | 0.13          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 18       | 0.13          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 18       | 0.13          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 18       | 0.13          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 18       | 0.13          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 18       | 0.13          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 18       | 0.13          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 23       | 0.13          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 23       | 0.13          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 23       | 0.13          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 23       | 0.13          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 23       | 0.13          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 23       | 0.13          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 37       | 0.13          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 37       | 0.13          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 37       | 0.13          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 37       | 0.13          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 37       | 0.13          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 37       | 0.13          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 38       | 0.13          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 38       | 0.13          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 38       | 0.13          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 38       | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 38       | 0.13          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 38       | 0.13          |
| (3,3203) | 1:42:A:TRP:HZ2 | 1:30:A:GLU:HA   | 17       | 0.13          |
| (3,3203) | 1:42:A:TRP:HZ2 | 1:30:A:GLU:HA   | 27       | 0.13          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 2        | 0.13          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 2        | 0.13          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 2        | 0.13          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 2        | 0.13          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 15       | 0.13          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 15       | 0.13          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 15       | 0.13          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 15       | 0.13          |
| (3,3191) | 1:43:A:TYR:HD1 | 1:44:A:LYS:H    | 28       | 0.13          |
| (3,3191) | 1:43:A:TYR:HD2 | 1:44:A:LYS:H    | 28       | 0.13          |
| (3,3191) | 1:43:A:TYR:HD1 | 1:44:A:LYS:H    | 29       | 0.13          |
| (3,3191) | 1:43:A:TYR:HD2 | 1:44:A:LYS:H    | 29       | 0.13          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 6        | 0.13          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 6        | 0.13          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 6        | 0.13          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 8        | 0.13          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 8        | 0.13          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 8        | 0.13          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 12       | 0.13          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 12       | 0.13          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 12       | 0.13          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 13       | 0.13          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 13       | 0.13          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 13       | 0.13          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 40       | 0.13          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 40       | 0.13          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 40       | 0.13          |
| (3,3175) | 1:69:A:HIS:HD2 | 1:69:A:HIS:HB3  | 21       | 0.13          |
| (3,3175) | 1:69:A:HIS:HD2 | 1:69:A:HIS:HB3  | 22       | 0.13          |
| (3,3175) | 1:69:A:HIS:HD2 | 1:69:A:HIS:HB3  | 23       | 0.13          |
| (3,3175) | 1:69:A:HIS:HD2 | 1:69:A:HIS:HB3  | 24       | 0.13          |
| (3,3175) | 1:69:A:HIS:HD2 | 1:69:A:HIS:HB3  | 25       | 0.13          |
| (3,3175) | 1:69:A:HIS:HD2 | 1:69:A:HIS:HB3  | 30       | 0.13          |
| (3,3143) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3  | 3        | 0.13          |
| (3,3143) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 3        | 0.13          |
| (3,3143) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3  | 17       | 0.13          |
| (3,3143) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 17       | 0.13          |
| (3,3143) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3  | 29       | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3143) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 29       | 0.13          |
| (3,3143) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3  | 37       | 0.13          |
| (3,3143) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 37       | 0.13          |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2  | 31       | 0.13          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2  | 31       | 0.13          |
| (3,3139) | 1:65:A:TYR:HE1 | 1:60:A:ASP:HB3  | 2        | 0.13          |
| (3,3139) | 1:65:A:TYR:HE2 | 1:60:A:ASP:HB3  | 2        | 0.13          |
| (3,3139) | 1:65:A:TYR:HE1 | 1:60:A:ASP:HB3  | 24       | 0.13          |
| (3,3139) | 1:65:A:TYR:HE2 | 1:60:A:ASP:HB3  | 24       | 0.13          |
| (3,3139) | 1:65:A:TYR:HE1 | 1:60:A:ASP:HB3  | 38       | 0.13          |
| (3,3139) | 1:65:A:TYR:HE2 | 1:60:A:ASP:HB3  | 38       | 0.13          |
| (3,3138) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB2  | 24       | 0.13          |
| (3,3138) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB2  | 24       | 0.13          |
| (3,3138) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB2  | 33       | 0.13          |
| (3,3138) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB2  | 33       | 0.13          |
| (3,3137) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3  | 4        | 0.13          |
| (3,3137) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3  | 4        | 0.13          |
| (3,3137) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3  | 11       | 0.13          |
| (3,3137) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3  | 11       | 0.13          |
| (3,3137) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3  | 35       | 0.13          |
| (3,3137) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3  | 35       | 0.13          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 6        | 0.13          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 6        | 0.13          |
| (3,3132) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 35       | 0.13          |
| (3,3132) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 35       | 0.13          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 6        | 0.13          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 6        | 0.13          |
| (3,3131) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 35       | 0.13          |
| (3,3131) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 35       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 7        | 0.13          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 7        | 0.13          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 7        | 0.13          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 7        | 0.13          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 7        | 0.13          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 7        | 0.13          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 10       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 10       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 10       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 10       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 10       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 10       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 12       | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 12       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 12       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 12       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 12       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 12       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 16       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 16       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 16       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 16       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 16       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 16       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 18       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 18       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 18       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 18       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 18       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 18       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 19       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 19       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 19       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 19       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 19       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 19       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 24       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 24       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 24       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 24       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 24       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 24       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 40       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 40       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 40       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 40       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 40       | 0.13          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 40       | 0.13          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 4        | 0.13          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 4        | 0.13          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 4        | 0.13          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 4        | 0.13          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 4        | 0.13          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 4        | 0.13          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 22       | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 22       | 0.13          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 22       | 0.13          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 22       | 0.13          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 22       | 0.13          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 22       | 0.13          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 31       | 0.13          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 31       | 0.13          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 31       | 0.13          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 31       | 0.13          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 31       | 0.13          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 31       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 3        | 0.13          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 3        | 0.13          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 3        | 0.13          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 3        | 0.13          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 9        | 0.13          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 9        | 0.13          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 9        | 0.13          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 9        | 0.13          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 10       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 10       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 10       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 10       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 12       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 12       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 12       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 12       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 14       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 14       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 14       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 14       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 21       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 21       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 21       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 21       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 23       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 23       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 23       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 23       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 27       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 27       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 27       | 0.13          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2 | 27       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1 | 28       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2 | 28       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1 | 28       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2 | 28       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1 | 36       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2 | 36       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1 | 36       | 0.13          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2 | 36       | 0.13          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1 | 14       | 0.13          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2 | 14       | 0.13          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1 | 14       | 0.13          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2 | 14       | 0.13          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1 | 14       | 0.13          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2 | 14       | 0.13          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1 | 22       | 0.13          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2 | 22       | 0.13          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1 | 22       | 0.13          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2 | 22       | 0.13          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1 | 22       | 0.13          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2 | 22       | 0.13          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1 | 25       | 0.13          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2 | 25       | 0.13          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1 | 25       | 0.13          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2 | 25       | 0.13          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1 | 25       | 0.13          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2 | 25       | 0.13          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1 | 27       | 0.13          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2 | 27       | 0.13          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1 | 27       | 0.13          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2 | 27       | 0.13          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1 | 27       | 0.13          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2 | 27       | 0.13          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1 | 32       | 0.13          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2 | 32       | 0.13          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1 | 32       | 0.13          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2 | 32       | 0.13          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1 | 32       | 0.13          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2 | 32       | 0.13          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1 | 35       | 0.13          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2 | 35       | 0.13          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1 | 35       | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 35       | 0.13          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 35       | 0.13          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 35       | 0.13          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 36       | 0.13          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 36       | 0.13          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 36       | 0.13          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 36       | 0.13          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 36       | 0.13          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 36       | 0.13          |
| (3,3092) | 1:7:A:ALA:HB1  | 1:88:A:ARG:HD3  | 20       | 0.13          |
| (3,3092) | 1:7:A:ALA:HB2  | 1:88:A:ARG:HD3  | 20       | 0.13          |
| (3,3092) | 1:7:A:ALA:HB3  | 1:88:A:ARG:HD3  | 20       | 0.13          |
| (3,3092) | 1:7:A:ALA:HB1  | 1:88:A:ARG:HD3  | 21       | 0.13          |
| (3,3092) | 1:7:A:ALA:HB2  | 1:88:A:ARG:HD3  | 21       | 0.13          |
| (3,3092) | 1:7:A:ALA:HB3  | 1:88:A:ARG:HD3  | 21       | 0.13          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 6        | 0.13          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 6        | 0.13          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 6        | 0.13          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 16       | 0.13          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 16       | 0.13          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 16       | 0.13          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 19       | 0.13          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 19       | 0.13          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 19       | 0.13          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 26       | 0.13          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 26       | 0.13          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 26       | 0.13          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 28       | 0.13          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 28       | 0.13          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 28       | 0.13          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 33       | 0.13          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 33       | 0.13          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 33       | 0.13          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 29       | 0.13          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 29       | 0.13          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 38       | 0.13          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 38       | 0.13          |
| (3,3041) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE1  | 14       | 0.13          |
| (3,3041) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE2  | 14       | 0.13          |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 25       | 0.13          |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 25       | 0.13          |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 34       | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 34       | 0.13          |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 38       | 0.13          |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 38       | 0.13          |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 40       | 0.13          |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 40       | 0.13          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 13       | 0.13          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 13       | 0.13          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 13       | 0.13          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 18       | 0.13          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 18       | 0.13          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 18       | 0.13          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 25       | 0.13          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 25       | 0.13          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 25       | 0.13          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 27       | 0.13          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 27       | 0.13          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 27       | 0.13          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 30       | 0.13          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 30       | 0.13          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 30       | 0.13          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 34       | 0.13          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 34       | 0.13          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 34       | 0.13          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 36       | 0.13          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 36       | 0.13          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 36       | 0.13          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 37       | 0.13          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 37       | 0.13          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 37       | 0.13          |
| (3,3019) | 1:30:A:GLU:HB2 | 1:14:A:LYS:HE2  | 10       | 0.13          |
| (3,3019) | 1:30:A:GLU:HB2 | 1:14:A:LYS:HE2  | 21       | 0.13          |
| (3,3019) | 1:30:A:GLU:HB2 | 1:14:A:LYS:HE2  | 38       | 0.13          |
| (3,3019) | 1:30:A:GLU:HB2 | 1:14:A:LYS:HE2  | 39       | 0.13          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 6        | 0.13          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 6        | 0.13          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 6        | 0.13          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 39       | 0.13          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 39       | 0.13          |
| (3,3012) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 39       | 0.13          |
| (3,2982) | 1:65:A:TYR:HA  | 1:42:A:TRP:HZ2  | 3        | 0.13          |
| (3,2982) | 1:65:A:TYR:HA  | 1:42:A:TRP:HZ2  | 12       | 0.13          |
| (3,2982) | 1:65:A:TYR:HA  | 1:42:A:TRP:HZ2  | 19       | 0.13          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,2982) | 1:65:A:TYR:HA  | 1:42:A:TRP:HZ2 | 21       | 0.13          |
| (3,2982) | 1:65:A:TYR:HA  | 1:42:A:TRP:HZ2 | 24       | 0.13          |
| (3,2982) | 1:65:A:TYR:HA  | 1:42:A:TRP:HZ2 | 33       | 0.13          |
| (3,2975) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD2 | 2        | 0.13          |
| (3,2975) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD2 | 20       | 0.13          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 2        | 0.13          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 3        | 0.13          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 4        | 0.13          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 5        | 0.13          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 6        | 0.13          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 7        | 0.13          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 8        | 0.13          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 10       | 0.13          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 12       | 0.13          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 13       | 0.13          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 14       | 0.13          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 18       | 0.13          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 19       | 0.13          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 20       | 0.13          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 21       | 0.13          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 23       | 0.13          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 24       | 0.13          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 26       | 0.13          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 27       | 0.13          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 28       | 0.13          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 29       | 0.13          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 30       | 0.13          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 32       | 0.13          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 33       | 0.13          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 34       | 0.13          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 35       | 0.13          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 36       | 0.13          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 39       | 0.13          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 40       | 0.13          |
| (3,2957) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 1        | 0.13          |
| (3,2957) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 4        | 0.13          |
| (3,2957) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 5        | 0.13          |
| (3,2957) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 7        | 0.13          |
| (3,2957) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 8        | 0.13          |
| (3,2957) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 10       | 0.13          |
| (3,2957) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 13       | 0.13          |
| (3,2957) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 14       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2957) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 17       | 0.13          |
| (3,2957) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 21       | 0.13          |
| (3,2957) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 23       | 0.13          |
| (3,2957) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 28       | 0.13          |
| (3,2957) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 33       | 0.13          |
| (3,2957) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 34       | 0.13          |
| (3,2957) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 37       | 0.13          |
| (3,2957) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 39       | 0.13          |
| (3,2944) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD1  | 3        | 0.13          |
| (3,2944) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD2  | 3        | 0.13          |
| (3,2944) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD1  | 17       | 0.13          |
| (3,2944) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD2  | 17       | 0.13          |
| (3,2944) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD1  | 29       | 0.13          |
| (3,2944) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD2  | 29       | 0.13          |
| (3,2944) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD1  | 37       | 0.13          |
| (3,2944) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD2  | 37       | 0.13          |
| (3,2938) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 4        | 0.13          |
| (3,2938) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 8        | 0.13          |
| (3,2938) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 31       | 0.13          |
| (3,2938) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 36       | 0.13          |
| (3,2936) | 1:17:A:GLN:HG2  | 1:17:A:GLN:H    | 28       | 0.13          |
| (3,2936) | 1:17:A:GLN:HG2  | 1:17:A:GLN:H    | 29       | 0.13          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 4        | 0.13          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 7        | 0.13          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 10       | 0.13          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 11       | 0.13          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 12       | 0.13          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 17       | 0.13          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 21       | 0.13          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 36       | 0.13          |
| (3,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 38       | 0.13          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 7        | 0.13          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 20       | 0.13          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 21       | 0.13          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 24       | 0.13          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 25       | 0.13          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 28       | 0.13          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 30       | 0.13          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 32       | 0.13          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 38       | 0.13          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 5        | 0.13          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 10       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 11       | 0.13          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 19       | 0.13          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 23       | 0.13          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 26       | 0.13          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 27       | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 1        | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 3        | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 5        | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 7        | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 8        | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 9        | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 10       | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 12       | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 13       | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 14       | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 15       | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 16       | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 17       | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 18       | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 19       | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 20       | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 21       | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 22       | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 23       | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 24       | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 25       | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 26       | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 27       | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 28       | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 30       | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 32       | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 35       | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 36       | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 37       | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 38       | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 39       | 0.13          |
| (3,2774) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 40       | 0.13          |
| (3,2761) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 11       | 0.13          |
| (3,2761) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 14       | 0.13          |
| (3,2761) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 31       | 0.13          |
| (3,2748) | 1:86:A:GLU:HG3  | 1:87:A:PRO:HA   | 17       | 0.13          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H    | 9        | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,2717) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3  | 7        | 0.13          |
| (3,2717) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3  | 8        | 0.13          |
| (3,2703) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA   | 4        | 0.13          |
| (3,2703) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA   | 14       | 0.13          |
| (3,2703) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA   | 33       | 0.13          |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 13       | 0.13          |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 14       | 0.13          |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 17       | 0.13          |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 21       | 0.13          |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 22       | 0.13          |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 24       | 0.13          |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 28       | 0.13          |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 35       | 0.13          |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 38       | 0.13          |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 39       | 0.13          |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 40       | 0.13          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 4        | 0.13          |
| (3,2679) | 1:25:A:GLN:HG3 | 1:26:A:SER:H    | 13       | 0.13          |
| (3,2679) | 1:25:A:GLN:HG3 | 1:26:A:SER:H    | 19       | 0.13          |
| (3,2679) | 1:25:A:GLN:HG3 | 1:26:A:SER:H    | 22       | 0.13          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 20       | 0.13          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 20       | 0.13          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 20       | 0.13          |
| (3,2653) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 9        | 0.13          |
| (3,2554) | 1:92:A:ARG:HA  | 1:83:A:ALA:H    | 29       | 0.13          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA   | 2        | 0.13          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA   | 8        | 0.13          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA   | 12       | 0.13          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA   | 17       | 0.13          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA   | 20       | 0.13          |
| (3,2541) | 1:73:A:PRO:HG3 | 1:73:A:PRO:HA   | 27       | 0.13          |
| (3,2541) | 1:73:A:PRO:HG3 | 1:73:A:PRO:HA   | 29       | 0.13          |
| (3,2541) | 1:73:A:PRO:HG3 | 1:73:A:PRO:HA   | 34       | 0.13          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA    | 31       | 0.13          |
| (3,2490) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HA    | 28       | 0.13          |
| (3,2482) | 1:9:A:PRO:HD2  | 1:8:A:GLU:HA    | 13       | 0.13          |
| (3,2482) | 1:9:A:PRO:HD2  | 1:8:A:GLU:HA    | 15       | 0.13          |
| (3,2463) | 1:4:A:PRO:HD3  | 1:3:A:ASP:HA    | 16       | 0.13          |
| (3,2463) | 1:4:A:PRO:HD3  | 1:3:A:ASP:HA    | 26       | 0.13          |
| (3,2434) | 1:82:A:ILE:HB  | 1:41:A:THR:H    | 8        | 0.13          |
| (3,2434) | 1:82:A:ILE:HB  | 1:41:A:THR:H    | 32       | 0.13          |
| (3,2434) | 1:82:A:ILE:HB  | 1:41:A:THR:H    | 40       | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,2419) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 6        | 0.13          |
| (3,2419) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 18       | 0.13          |
| (3,2419) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 20       | 0.13          |
| (3,2419) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 23       | 0.13          |
| (3,2412) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2  | 22       | 0.13          |
| (3,2412) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2  | 29       | 0.13          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ   | 7        | 0.13          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ   | 7        | 0.13          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ   | 7        | 0.13          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ   | 10       | 0.13          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ   | 10       | 0.13          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ   | 10       | 0.13          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ   | 39       | 0.13          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ   | 39       | 0.13          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ   | 39       | 0.13          |
| (3,2342) | 1:26:A:SER:HB3 | 1:27:A:ALA:H    | 4        | 0.13          |
| (3,2342) | 1:26:A:SER:HB3 | 1:27:A:ALA:H    | 25       | 0.13          |
| (3,2334) | 1:26:A:SER:HA  | 1:68:A:ILE:HG21 | 31       | 0.13          |
| (3,2334) | 1:26:A:SER:HA  | 1:68:A:ILE:HG22 | 31       | 0.13          |
| (3,2334) | 1:26:A:SER:HA  | 1:68:A:ILE:HG23 | 31       | 0.13          |
| (3,2290) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H    | 2        | 0.13          |
| (3,2290) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H    | 3        | 0.13          |
| (3,2290) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H    | 6        | 0.13          |
| (3,2290) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H    | 9        | 0.13          |
| (3,2290) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H    | 14       | 0.13          |
| (3,2290) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H    | 19       | 0.13          |
| (3,2290) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H    | 25       | 0.13          |
| (3,2290) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H    | 31       | 0.13          |
| (3,2290) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H    | 33       | 0.13          |
| (3,2290) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H    | 35       | 0.13          |
| (3,2290) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H    | 37       | 0.13          |
| (3,2268) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG21 | 2        | 0.13          |
| (3,2268) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG22 | 2        | 0.13          |
| (3,2268) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG23 | 2        | 0.13          |
| (3,2268) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG21 | 17       | 0.13          |
| (3,2268) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG22 | 17       | 0.13          |
| (3,2268) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG23 | 17       | 0.13          |
| (3,2268) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG21 | 21       | 0.13          |
| (3,2268) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG22 | 21       | 0.13          |
| (3,2268) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG23 | 21       | 0.13          |
| (3,2268) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG21 | 23       | 0.13          |
| (3,2268) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG22 | 23       | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,2268) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG23 | 23       | 0.13          |
| (3,2268) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG21 | 38       | 0.13          |
| (3,2268) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG22 | 38       | 0.13          |
| (3,2268) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG23 | 38       | 0.13          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 27       | 0.13          |
| (3,2253) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 27       | 0.13          |
| (3,2240) | 1:18:A:ASN:HB2 | 1:18:A:ASN:H    | 6        | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 1        | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 2        | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 3        | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 4        | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 5        | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 6        | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 7        | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 8        | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 9        | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 10       | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 11       | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 12       | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 13       | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 14       | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 15       | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 17       | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 18       | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 19       | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 20       | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 21       | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 22       | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 23       | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 24       | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 25       | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 26       | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 27       | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 28       | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 29       | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 30       | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 31       | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 32       | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 34       | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 35       | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 36       | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 37       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2153) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 38       | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 39       | 0.13          |
| (3,2153) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 40       | 0.13          |
| (3,2148) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 2        | 0.13          |
| (3,2148) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 30       | 0.13          |
| (3,2148) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 35       | 0.13          |
| (3,2148) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 38       | 0.13          |
| (3,2139) | 1:67:A:THR:HB   | 1:56:A:ASN:HB2  | 19       | 0.13          |
| (3,2102) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HA   | 37       | 0.13          |
| (3,2102) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HA   | 37       | 0.13          |
| (3,2102) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HA   | 37       | 0.13          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 9        | 0.13          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 9        | 0.13          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 9        | 0.13          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 20       | 0.13          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 20       | 0.13          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 20       | 0.13          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1  | 20       | 0.13          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2  | 20       | 0.13          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1  | 20       | 0.13          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2  | 20       | 0.13          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1  | 20       | 0.13          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2  | 20       | 0.13          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1  | 32       | 0.13          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2  | 32       | 0.13          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1  | 32       | 0.13          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2  | 32       | 0.13          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1  | 32       | 0.13          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2  | 32       | 0.13          |
| (3,2081) | 1:97:A:LEU:HD11 | 1:21:A:VAL:HB   | 7        | 0.13          |
| (3,2081) | 1:97:A:LEU:HD12 | 1:21:A:VAL:HB   | 7        | 0.13          |
| (3,2081) | 1:97:A:LEU:HD13 | 1:21:A:VAL:HB   | 7        | 0.13          |
| (3,2081) | 1:97:A:LEU:HD11 | 1:21:A:VAL:HB   | 34       | 0.13          |
| (3,2081) | 1:97:A:LEU:HD12 | 1:21:A:VAL:HB   | 34       | 0.13          |
| (3,2081) | 1:97:A:LEU:HD13 | 1:21:A:VAL:HB   | 34       | 0.13          |
| (3,2073) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 17       | 0.13          |
| (3,2073) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 17       | 0.13          |
| (3,2073) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 17       | 0.13          |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD11 | 1        | 0.13          |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD12 | 1        | 0.13          |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD13 | 1        | 0.13          |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD11 | 1        | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD12 | 1        | 0.13          |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD13 | 1        | 0.13          |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD11 | 1        | 0.13          |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD12 | 1        | 0.13          |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD13 | 1        | 0.13          |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD11 | 10       | 0.13          |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD12 | 10       | 0.13          |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD13 | 10       | 0.13          |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD11 | 10       | 0.13          |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD12 | 10       | 0.13          |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD13 | 10       | 0.13          |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD11 | 10       | 0.13          |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD12 | 10       | 0.13          |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD13 | 10       | 0.13          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD21 | 34       | 0.13          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD22 | 34       | 0.13          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD23 | 34       | 0.13          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD21 | 34       | 0.13          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD22 | 34       | 0.13          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD23 | 34       | 0.13          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD21 | 34       | 0.13          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD22 | 34       | 0.13          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD23 | 34       | 0.13          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1  | 10       | 0.13          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2  | 10       | 0.13          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1  | 10       | 0.13          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2  | 10       | 0.13          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1  | 10       | 0.13          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2  | 10       | 0.13          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 20       | 0.13          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 20       | 0.13          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 20       | 0.13          |
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3  | 1        | 0.13          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3  | 1        | 0.13          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3  | 1        | 0.13          |
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3  | 12       | 0.13          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3  | 12       | 0.13          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3  | 12       | 0.13          |
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3  | 30       | 0.13          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3  | 30       | 0.13          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3  | 30       | 0.13          |
| (3,2019) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD1  | 35       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2019) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD2  | 35       | 0.13          |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1  | 18       | 0.13          |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2  | 18       | 0.13          |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3  | 18       | 0.13          |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1  | 18       | 0.13          |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2  | 18       | 0.13          |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3  | 18       | 0.13          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1  | 18       | 0.13          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2  | 18       | 0.13          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3  | 18       | 0.13          |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1  | 28       | 0.13          |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2  | 28       | 0.13          |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3  | 28       | 0.13          |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1  | 28       | 0.13          |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2  | 28       | 0.13          |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3  | 28       | 0.13          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1  | 28       | 0.13          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2  | 28       | 0.13          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3  | 28       | 0.13          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 2        | 0.13          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 18       | 0.13          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 19       | 0.13          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 33       | 0.13          |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 3        | 0.13          |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 3        | 0.13          |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 3        | 0.13          |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 15       | 0.13          |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 15       | 0.13          |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 15       | 0.13          |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 28       | 0.13          |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 28       | 0.13          |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 28       | 0.13          |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 29       | 0.13          |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 29       | 0.13          |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 29       | 0.13          |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 39       | 0.13          |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 39       | 0.13          |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 39       | 0.13          |
| (3,1997) | 1:21:A:VAL:HG11 | 1:25:A:GLN:HG3  | 27       | 0.13          |
| (3,1997) | 1:21:A:VAL:HG12 | 1:25:A:GLN:HG3  | 27       | 0.13          |
| (3,1997) | 1:21:A:VAL:HG13 | 1:25:A:GLN:HG3  | 27       | 0.13          |
| (3,1993) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 3        | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1993) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 3        | 0.13          |
| (3,1993) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 3        | 0.13          |
| (3,1993) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 11       | 0.13          |
| (3,1993) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 11       | 0.13          |
| (3,1993) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 11       | 0.13          |
| (3,1993) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 21       | 0.13          |
| (3,1993) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 21       | 0.13          |
| (3,1993) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 21       | 0.13          |
| (3,1993) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 23       | 0.13          |
| (3,1993) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 23       | 0.13          |
| (3,1993) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 23       | 0.13          |
| (3,1993) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 25       | 0.13          |
| (3,1993) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 25       | 0.13          |
| (3,1993) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 25       | 0.13          |
| (3,1993) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 26       | 0.13          |
| (3,1993) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 26       | 0.13          |
| (3,1993) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 26       | 0.13          |
| (3,1993) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 34       | 0.13          |
| (3,1993) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 34       | 0.13          |
| (3,1993) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 34       | 0.13          |
| (3,1993) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 36       | 0.13          |
| (3,1993) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 36       | 0.13          |
| (3,1993) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 36       | 0.13          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 11       | 0.13          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 29       | 0.13          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H    | 7        | 0.13          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H    | 7        | 0.13          |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H    | 7        | 0.13          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H    | 13       | 0.13          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H    | 13       | 0.13          |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H    | 13       | 0.13          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H    | 20       | 0.13          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H    | 20       | 0.13          |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H    | 20       | 0.13          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H    | 21       | 0.13          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H    | 21       | 0.13          |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H    | 21       | 0.13          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H    | 23       | 0.13          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H    | 23       | 0.13          |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H    | 23       | 0.13          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H    | 25       | 0.13          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H    | 25       | 0.13          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 25       | 0.13          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 35       | 0.13          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 35       | 0.13          |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 35       | 0.13          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 36       | 0.13          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 36       | 0.13          |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 36       | 0.13          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 38       | 0.13          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 38       | 0.13          |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 38       | 0.13          |
| (3,1906) | 1:66:A:MET:HE1  | 1:79:A:TYR:HA  | 10       | 0.13          |
| (3,1906) | 1:66:A:MET:HE2  | 1:79:A:TYR:HA  | 10       | 0.13          |
| (3,1906) | 1:66:A:MET:HE3  | 1:79:A:TYR:HA  | 10       | 0.13          |
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 3        | 0.13          |
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 3        | 0.13          |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 3        | 0.13          |
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 35       | 0.13          |
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 35       | 0.13          |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 35       | 0.13          |
| (3,1899) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3 | 26       | 0.13          |
| (3,1899) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3 | 26       | 0.13          |
| (3,1899) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3 | 26       | 0.13          |
| (3,1864) | 1:7:A:ALA:HB1   | 1:88:A:ARG:HA  | 13       | 0.13          |
| (3,1864) | 1:7:A:ALA:HB2   | 1:88:A:ARG:HA  | 13       | 0.13          |
| (3,1864) | 1:7:A:ALA:HB3   | 1:88:A:ARG:HA  | 13       | 0.13          |
| (3,1864) | 1:7:A:ALA:HB1   | 1:88:A:ARG:HA  | 19       | 0.13          |
| (3,1864) | 1:7:A:ALA:HB2   | 1:88:A:ARG:HA  | 19       | 0.13          |
| (3,1864) | 1:7:A:ALA:HB3   | 1:88:A:ARG:HA  | 19       | 0.13          |
| (3,1864) | 1:7:A:ALA:HB1   | 1:88:A:ARG:HA  | 30       | 0.13          |
| (3,1864) | 1:7:A:ALA:HB2   | 1:88:A:ARG:HA  | 30       | 0.13          |
| (3,1864) | 1:7:A:ALA:HB3   | 1:88:A:ARG:HA  | 30       | 0.13          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 6        | 0.13          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 6        | 0.13          |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 6        | 0.13          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 15       | 0.13          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 15       | 0.13          |
| (3,1856) | 1:27:A:ALA:HB3  | 1:28:A:THR:H   | 15       | 0.13          |
| (3,1814) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 2        | 0.13          |
| (3,1814) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 6        | 0.13          |
| (3,1814) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 8        | 0.13          |
| (3,1814) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 11       | 0.13          |
| (3,1814) | 1:98:A:LYS:HD2  | 1:98:A:LYS:HG2 | 16       | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,1814) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 18       | 0.13          |
| (3,1814) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 26       | 0.13          |
| (3,1814) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 27       | 0.13          |
| (3,1814) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 28       | 0.13          |
| (3,1814) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 33       | 0.13          |
| (3,1814) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2  | 37       | 0.13          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 2        | 0.13          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 3        | 0.13          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 4        | 0.13          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 5        | 0.13          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 6        | 0.13          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 7        | 0.13          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 8        | 0.13          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 10       | 0.13          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 12       | 0.13          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 13       | 0.13          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 14       | 0.13          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 18       | 0.13          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 19       | 0.13          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 20       | 0.13          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 21       | 0.13          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 23       | 0.13          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 24       | 0.13          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 26       | 0.13          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 27       | 0.13          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 28       | 0.13          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 29       | 0.13          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 30       | 0.13          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 32       | 0.13          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 33       | 0.13          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 34       | 0.13          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 35       | 0.13          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 36       | 0.13          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 39       | 0.13          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 40       | 0.13          |
| (3,1728) | 1:38:A:ALA:HB1 | 1:83:A:ALA:HA   | 34       | 0.13          |
| (3,1728) | 1:38:A:ALA:HB2 | 1:83:A:ALA:HA   | 34       | 0.13          |
| (3,1728) | 1:38:A:ALA:HB3 | 1:83:A:ALA:HA   | 34       | 0.13          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG11 | 26       | 0.13          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG12 | 26       | 0.13          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG13 | 26       | 0.13          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG11 | 26       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG12 | 26       | 0.13          |
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 26       | 0.13          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 26       | 0.13          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 26       | 0.13          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 26       | 0.13          |
| (3,1721) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG11 | 32       | 0.13          |
| (3,1721) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG12 | 32       | 0.13          |
| (3,1721) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG13 | 32       | 0.13          |
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG11 | 32       | 0.13          |
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG12 | 32       | 0.13          |
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 32       | 0.13          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 32       | 0.13          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 32       | 0.13          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 32       | 0.13          |
| (3,1712) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 9        | 0.13          |
| (3,1712) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 9        | 0.13          |
| (3,1712) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 9        | 0.13          |
| (3,1712) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 11       | 0.13          |
| (3,1712) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 11       | 0.13          |
| (3,1712) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 11       | 0.13          |
| (3,1712) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 16       | 0.13          |
| (3,1712) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 16       | 0.13          |
| (3,1712) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 16       | 0.13          |
| (3,1712) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 17       | 0.13          |
| (3,1712) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 17       | 0.13          |
| (3,1712) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 17       | 0.13          |
| (3,1712) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 18       | 0.13          |
| (3,1712) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 18       | 0.13          |
| (3,1712) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 18       | 0.13          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 9        | 0.13          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 9        | 0.13          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 9        | 0.13          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 9        | 0.13          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 9        | 0.13          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 9        | 0.13          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 9        | 0.13          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 9        | 0.13          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 9        | 0.13          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 31       | 0.13          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 31       | 0.13          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 31       | 0.13          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 31       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 31       | 0.13          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 31       | 0.13          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 31       | 0.13          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 31       | 0.13          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 31       | 0.13          |
| (3,1683) | 1:85:A:LEU:HD11 | 1:35:A:PHE:HD1  | 16       | 0.13          |
| (3,1683) | 1:85:A:LEU:HD11 | 1:35:A:PHE:HD2  | 16       | 0.13          |
| (3,1683) | 1:85:A:LEU:HD12 | 1:35:A:PHE:HD1  | 16       | 0.13          |
| (3,1683) | 1:85:A:LEU:HD12 | 1:35:A:PHE:HD2  | 16       | 0.13          |
| (3,1683) | 1:85:A:LEU:HD13 | 1:35:A:PHE:HD1  | 16       | 0.13          |
| (3,1683) | 1:85:A:LEU:HD13 | 1:35:A:PHE:HD2  | 16       | 0.13          |
| (3,1654) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 11       | 0.13          |
| (3,1654) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 11       | 0.13          |
| (3,1654) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 11       | 0.13          |
| (3,1654) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 11       | 0.13          |
| (3,1654) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 11       | 0.13          |
| (3,1654) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 11       | 0.13          |
| (3,1654) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 11       | 0.13          |
| (3,1654) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 11       | 0.13          |
| (3,1654) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 11       | 0.13          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 1        | 0.13          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 1        | 0.13          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 1        | 0.13          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 1        | 0.13          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 1        | 0.13          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 1        | 0.13          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 1        | 0.13          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 1        | 0.13          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 1        | 0.13          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 35       | 0.13          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 35       | 0.13          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 35       | 0.13          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 35       | 0.13          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 35       | 0.13          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 35       | 0.13          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 35       | 0.13          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 35       | 0.13          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 35       | 0.13          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 4        | 0.13          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 4        | 0.13          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 4        | 0.13          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 6        | 0.13          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H   | 6        | 0.13          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 6        | 0.13          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H   | 9        | 0.13          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H   | 9        | 0.13          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 9        | 0.13          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H   | 10       | 0.13          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H   | 10       | 0.13          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 10       | 0.13          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H   | 16       | 0.13          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H   | 16       | 0.13          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 16       | 0.13          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H   | 17       | 0.13          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H   | 17       | 0.13          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 17       | 0.13          |
| (3,1628) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2 | 15       | 0.13          |
| (3,1628) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2 | 15       | 0.13          |
| (3,1628) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2 | 15       | 0.13          |
| (3,1628) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2 | 19       | 0.13          |
| (3,1628) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2 | 19       | 0.13          |
| (3,1628) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2 | 19       | 0.13          |
| (3,1627) | 1:82:A:ILE:HG21 | 1:84:A:ARG:HG2 | 6        | 0.13          |
| (3,1627) | 1:82:A:ILE:HG22 | 1:84:A:ARG:HG2 | 6        | 0.13          |
| (3,1627) | 1:82:A:ILE:HG23 | 1:84:A:ARG:HG2 | 6        | 0.13          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2 | 2        | 0.13          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 2        | 0.13          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 2        | 0.13          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2 | 35       | 0.13          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 35       | 0.13          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 35       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 7        | 0.13          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 7        | 0.13          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 7        | 0.13          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 7        | 0.13          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 7        | 0.13          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 7        | 0.13          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 10       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 10       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 10       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 10       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 10       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 10       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 12       | 0.13          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 12       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 12       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 12       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 12       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 12       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 16       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 16       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 16       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 16       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 16       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 16       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 18       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 18       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 18       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 18       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 18       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 18       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 19       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 19       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 19       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 19       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 19       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 19       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 24       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 24       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 24       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 24       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 24       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 24       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 40       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 40       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 40       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 40       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 40       | 0.13          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 40       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 8        | 0.13          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 8        | 0.13          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 8        | 0.13          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 8        | 0.13          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 8        | 0.13          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 8        | 0.13          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 12       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 12       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 12       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 12       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 12       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 12       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 18       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 18       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 18       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 18       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 18       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 18       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 21       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 21       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 21       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 21       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 21       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 21       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 23       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 23       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 23       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 23       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 23       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 23       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 33       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 33       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 33       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 33       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 33       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 33       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 40       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 40       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 40       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 40       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 40       | 0.13          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 40       | 0.13          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 15       | 0.13          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 15       | 0.13          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 15       | 0.13          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 18       | 0.13          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 18       | 0.13          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 18       | 0.13          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 24       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 24       | 0.13          |
| (3,1594) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 24       | 0.13          |
| (3,1554) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA    | 23       | 0.13          |
| (3,1554) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA    | 23       | 0.13          |
| (3,1554) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA    | 23       | 0.13          |
| (3,1554) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA    | 31       | 0.13          |
| (3,1554) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA    | 31       | 0.13          |
| (3,1554) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA    | 31       | 0.13          |
| (3,1554) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA    | 40       | 0.13          |
| (3,1554) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA    | 40       | 0.13          |
| (3,1554) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA    | 40       | 0.13          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H    | 1        | 0.13          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H    | 1        | 0.13          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H    | 1        | 0.13          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H    | 8        | 0.13          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H    | 8        | 0.13          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H    | 8        | 0.13          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H    | 13       | 0.13          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H    | 13       | 0.13          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H    | 13       | 0.13          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H    | 14       | 0.13          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H    | 14       | 0.13          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H    | 14       | 0.13          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H    | 15       | 0.13          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H    | 15       | 0.13          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H    | 15       | 0.13          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H    | 21       | 0.13          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H    | 21       | 0.13          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H    | 21       | 0.13          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H    | 22       | 0.13          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H    | 22       | 0.13          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H    | 22       | 0.13          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H    | 27       | 0.13          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H    | 27       | 0.13          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H    | 27       | 0.13          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H    | 28       | 0.13          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H    | 28       | 0.13          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H    | 28       | 0.13          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H    | 35       | 0.13          |
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H    | 35       | 0.13          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H    | 35       | 0.13          |
| (3,1542) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H    | 40       | 0.13          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1542) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H   | 40       | 0.13          |
| (3,1542) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H   | 40       | 0.13          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 10       | 0.13          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 10       | 0.13          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 10       | 0.13          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 12       | 0.13          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 12       | 0.13          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 12       | 0.13          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 21       | 0.13          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 21       | 0.13          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 21       | 0.13          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 24       | 0.13          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 24       | 0.13          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 24       | 0.13          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 27       | 0.13          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 27       | 0.13          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 27       | 0.13          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 28       | 0.13          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 28       | 0.13          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 28       | 0.13          |
| (3,1517) | 1:66:A:MET:HE1  | 1:29:A:PHE:H   | 8        | 0.13          |
| (3,1517) | 1:66:A:MET:HE2  | 1:29:A:PHE:H   | 8        | 0.13          |
| (3,1517) | 1:66:A:MET:HE3  | 1:29:A:PHE:H   | 8        | 0.13          |
| (3,1517) | 1:66:A:MET:HE1  | 1:29:A:PHE:H   | 11       | 0.13          |
| (3,1517) | 1:66:A:MET:HE2  | 1:29:A:PHE:H   | 11       | 0.13          |
| (3,1517) | 1:66:A:MET:HE3  | 1:29:A:PHE:H   | 11       | 0.13          |
| (3,1517) | 1:66:A:MET:HE1  | 1:29:A:PHE:H   | 38       | 0.13          |
| (3,1517) | 1:66:A:MET:HE2  | 1:29:A:PHE:H   | 38       | 0.13          |
| (3,1517) | 1:66:A:MET:HE3  | 1:29:A:PHE:H   | 38       | 0.13          |
| (3,1514) | 1:66:A:MET:HE1  | 1:42:A:TRP:HE1 | 6        | 0.13          |
| (3,1514) | 1:66:A:MET:HE2  | 1:42:A:TRP:HE1 | 6        | 0.13          |
| (3,1514) | 1:66:A:MET:HE3  | 1:42:A:TRP:HE1 | 6        | 0.13          |
| (3,1514) | 1:66:A:MET:HE1  | 1:42:A:TRP:HE1 | 8        | 0.13          |
| (3,1514) | 1:66:A:MET:HE2  | 1:42:A:TRP:HE1 | 8        | 0.13          |
| (3,1514) | 1:66:A:MET:HE3  | 1:42:A:TRP:HE1 | 8        | 0.13          |
| (3,1514) | 1:66:A:MET:HE1  | 1:42:A:TRP:HE1 | 12       | 0.13          |
| (3,1514) | 1:66:A:MET:HE2  | 1:42:A:TRP:HE1 | 12       | 0.13          |
| (3,1514) | 1:66:A:MET:HE3  | 1:42:A:TRP:HE1 | 12       | 0.13          |
| (3,1514) | 1:66:A:MET:HE1  | 1:42:A:TRP:HE1 | 13       | 0.13          |
| (3,1514) | 1:66:A:MET:HE2  | 1:42:A:TRP:HE1 | 13       | 0.13          |
| (3,1514) | 1:66:A:MET:HE3  | 1:42:A:TRP:HE1 | 13       | 0.13          |
| (3,1514) | 1:66:A:MET:HE1  | 1:42:A:TRP:HE1 | 40       | 0.13          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,1514) | 1:66:A:MET:HE2 | 1:42:A:TRP:HE1 | 40       | 0.13          |
| (3,1514) | 1:66:A:MET:HE3 | 1:42:A:TRP:HE1 | 40       | 0.13          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 2        | 0.13          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 2        | 0.13          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 2        | 0.13          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 2        | 0.13          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 2        | 0.13          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 2        | 0.13          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 10       | 0.13          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 10       | 0.13          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 10       | 0.13          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 10       | 0.13          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 10       | 0.13          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 10       | 0.13          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 18       | 0.13          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 18       | 0.13          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 18       | 0.13          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 18       | 0.13          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 18       | 0.13          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 18       | 0.13          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 24       | 0.13          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 24       | 0.13          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 24       | 0.13          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 24       | 0.13          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 24       | 0.13          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 24       | 0.13          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 28       | 0.13          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 28       | 0.13          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 28       | 0.13          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 28       | 0.13          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 28       | 0.13          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 28       | 0.13          |
| (3,1512) | 1:66:A:MET:HE1 | 1:42:A:TRP:HZ3 | 4        | 0.13          |
| (3,1512) | 1:66:A:MET:HE2 | 1:42:A:TRP:HZ3 | 4        | 0.13          |
| (3,1512) | 1:66:A:MET:HE3 | 1:42:A:TRP:HZ3 | 4        | 0.13          |
| (3,1512) | 1:66:A:MET:HE1 | 1:42:A:TRP:HZ3 | 14       | 0.13          |
| (3,1512) | 1:66:A:MET:HE2 | 1:42:A:TRP:HZ3 | 14       | 0.13          |
| (3,1512) | 1:66:A:MET:HE3 | 1:42:A:TRP:HZ3 | 14       | 0.13          |
| (3,1512) | 1:66:A:MET:HE1 | 1:42:A:TRP:HZ3 | 17       | 0.13          |
| (3,1512) | 1:66:A:MET:HE2 | 1:42:A:TRP:HZ3 | 17       | 0.13          |
| (3,1512) | 1:66:A:MET:HE3 | 1:42:A:TRP:HZ3 | 17       | 0.13          |
| (3,1511) | 1:66:A:MET:HE1 | 1:42:A:TRP:HB2 | 8        | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1511) | 1:66:A:MET:HE2  | 1:42:A:TRP:HB2  | 8        | 0.13          |
| (3,1511) | 1:66:A:MET:HE3  | 1:42:A:TRP:HB2  | 8        | 0.13          |
| (3,1511) | 1:66:A:MET:HE1  | 1:42:A:TRP:HB2  | 17       | 0.13          |
| (3,1511) | 1:66:A:MET:HE2  | 1:42:A:TRP:HB2  | 17       | 0.13          |
| (3,1511) | 1:66:A:MET:HE3  | 1:42:A:TRP:HB2  | 17       | 0.13          |
| (3,1511) | 1:66:A:MET:HE1  | 1:42:A:TRP:HB2  | 36       | 0.13          |
| (3,1511) | 1:66:A:MET:HE2  | 1:42:A:TRP:HB2  | 36       | 0.13          |
| (3,1511) | 1:66:A:MET:HE3  | 1:42:A:TRP:HB2  | 36       | 0.13          |
| (3,1506) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD11 | 3        | 0.13          |
| (3,1506) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD12 | 3        | 0.13          |
| (3,1506) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD13 | 3        | 0.13          |
| (3,1506) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD11 | 3        | 0.13          |
| (3,1506) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD12 | 3        | 0.13          |
| (3,1506) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD13 | 3        | 0.13          |
| (3,1506) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD11 | 3        | 0.13          |
| (3,1506) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD12 | 3        | 0.13          |
| (3,1506) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD13 | 3        | 0.13          |
| (3,1498) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 14       | 0.13          |
| (3,1498) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 14       | 0.13          |
| (3,1498) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 14       | 0.13          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA   | 14       | 0.13          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA   | 14       | 0.13          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA   | 14       | 0.13          |
| (3,1496) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA   | 18       | 0.13          |
| (3,1496) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA   | 18       | 0.13          |
| (3,1496) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA   | 18       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H    | 3        | 0.13          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H    | 3        | 0.13          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H    | 3        | 0.13          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H    | 6        | 0.13          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H    | 6        | 0.13          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H    | 6        | 0.13          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H    | 7        | 0.13          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H    | 7        | 0.13          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H    | 7        | 0.13          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H    | 8        | 0.13          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H    | 8        | 0.13          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H    | 8        | 0.13          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H    | 11       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H    | 11       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H    | 11       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H    | 12       | 0.13          |

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| Key      | Atom-1          | Atom-2       | Model ID | Violation (Å) |
|----------|-----------------|--------------|----------|---------------|
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 12       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 12       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 13       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 13       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 13       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 14       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 14       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 14       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 16       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 16       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 16       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 17       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 17       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 17       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 19       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 19       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 19       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 21       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 21       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 21       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 23       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 23       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 23       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 24       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 24       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 24       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 25       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 25       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 25       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 29       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 29       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 29       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 30       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 30       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 30       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 33       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 33       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 33       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 34       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 34       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 34       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 36       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H    | 36       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H    | 36       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H    | 37       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H    | 37       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H    | 37       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H    | 38       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H    | 38       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H    | 38       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H    | 40       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H    | 40       | 0.13          |
| (3,1480) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H    | 40       | 0.13          |
| (3,1412) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HA  | 5        | 0.13          |
| (3,1412) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HA  | 5        | 0.13          |
| (3,1412) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HA  | 5        | 0.13          |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H    | 6        | 0.13          |
| (3,1407) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H    | 6        | 0.13          |
| (3,1407) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H    | 6        | 0.13          |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H    | 17       | 0.13          |
| (3,1407) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H    | 17       | 0.13          |
| (3,1407) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H    | 17       | 0.13          |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H    | 20       | 0.13          |
| (3,1407) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H    | 20       | 0.13          |
| (3,1407) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H    | 20       | 0.13          |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H    | 31       | 0.13          |
| (3,1407) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H    | 31       | 0.13          |
| (3,1407) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H    | 31       | 0.13          |
| (3,1405) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H    | 3        | 0.13          |
| (3,1405) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H    | 3        | 0.13          |
| (3,1405) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H    | 3        | 0.13          |
| (3,1405) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H    | 13       | 0.13          |
| (3,1405) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H    | 13       | 0.13          |
| (3,1405) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H    | 13       | 0.13          |
| (3,1405) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H    | 19       | 0.13          |
| (3,1405) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H    | 19       | 0.13          |
| (3,1405) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H    | 19       | 0.13          |
| (3,1405) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H    | 40       | 0.13          |
| (3,1405) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H    | 40       | 0.13          |
| (3,1405) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H    | 40       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB1  | 1:16:A:ILE:HG12 | 7        | 0.13          |
| (3,1404) | 1:95:A:ALA:HB2  | 1:16:A:ILE:HG12 | 7        | 0.13          |
| (3,1404) | 1:95:A:ALA:HB3  | 1:16:A:ILE:HG12 | 7        | 0.13          |
| (3,1404) | 1:95:A:ALA:HB1  | 1:16:A:ILE:HG12 | 10       | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 10       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 10       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 11       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 11       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 11       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 13       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 13       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 13       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 15       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 15       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 15       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 17       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 17       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 17       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 24       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 24       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 24       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 26       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 26       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 26       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 28       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 28       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 28       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 33       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 33       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 33       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 34       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 34       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 34       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 38       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 38       | 0.13          |
| (3,1404) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 38       | 0.13          |
| (3,1391) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ   | 4        | 0.13          |
| (3,1391) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ   | 4        | 0.13          |
| (3,1391) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ   | 4        | 0.13          |
| (3,1391) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ   | 21       | 0.13          |
| (3,1391) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ   | 21       | 0.13          |
| (3,1391) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ   | 21       | 0.13          |
| (3,1391) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ   | 30       | 0.13          |
| (3,1391) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ   | 30       | 0.13          |
| (3,1391) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ   | 30       | 0.13          |
| (3,1391) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ   | 31       | 0.13          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,1391) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ  | 31       | 0.13          |
| (3,1391) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ  | 31       | 0.13          |
| (3,1391) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ  | 39       | 0.13          |
| (3,1391) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ  | 39       | 0.13          |
| (3,1391) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ  | 39       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 6        | 0.13          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 6        | 0.13          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 6        | 0.13          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 6        | 0.13          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 6        | 0.13          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 6        | 0.13          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 6        | 0.13          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 6        | 0.13          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 6        | 0.13          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 25       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 25       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 25       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 25       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 25       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 25       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 25       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 25       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 25       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 33       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 33       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 33       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 33       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 33       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 33       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 33       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 33       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 33       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 34       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 34       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 34       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 34       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 34       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 34       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 34       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 34       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 34       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 35       | 0.13          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 35       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 35       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 35       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 35       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 35       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 35       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 35       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 35       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 39       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 39       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 39       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 39       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 39       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 39       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 39       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 39       | 0.13          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 39       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 6        | 0.13          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 6        | 0.13          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 6        | 0.13          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 6        | 0.13          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 6        | 0.13          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 6        | 0.13          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 6        | 0.13          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 6        | 0.13          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 6        | 0.13          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 25       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 25       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 25       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 25       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 25       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 25       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 25       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 25       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 25       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 33       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 33       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 33       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 33       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 33       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 33       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 33       | 0.13          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB2 | 33       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB3 | 33       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB1 | 34       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB2 | 34       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB3 | 34       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB1 | 34       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB2 | 34       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB3 | 34       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB1 | 34       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB2 | 34       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB3 | 34       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB1 | 35       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB2 | 35       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB3 | 35       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB1 | 35       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB2 | 35       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB3 | 35       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB1 | 35       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB2 | 35       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB3 | 35       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB1 | 39       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB2 | 39       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB3 | 39       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB1 | 39       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB2 | 39       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB3 | 39       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB1 | 39       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB2 | 39       | 0.13          |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB3 | 39       | 0.13          |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3 | 9        | 0.13          |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3 | 12       | 0.13          |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3 | 29       | 0.13          |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3 | 34       | 0.13          |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3 | 39       | 0.13          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA  | 1        | 0.13          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA  | 1        | 0.13          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA  | 1        | 0.13          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA  | 28       | 0.13          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA  | 28       | 0.13          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA  | 28       | 0.13          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H   | 1        | 0.13          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H   | 3        | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 5        | 0.13          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 6        | 0.13          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 7        | 0.13          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 8        | 0.13          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 9        | 0.13          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 12       | 0.13          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 13       | 0.13          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 21       | 0.13          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 24       | 0.13          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 27       | 0.13          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 38       | 0.13          |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 4        | 0.13          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 28       | 0.13          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 28       | 0.13          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 28       | 0.13          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 29       | 0.13          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 29       | 0.13          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 29       | 0.13          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1  | 18       | 0.13          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2  | 18       | 0.13          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3  | 18       | 0.13          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1  | 18       | 0.13          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2  | 18       | 0.13          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3  | 18       | 0.13          |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1  | 18       | 0.13          |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2  | 18       | 0.13          |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3  | 18       | 0.13          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1  | 28       | 0.13          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2  | 28       | 0.13          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3  | 28       | 0.13          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1  | 28       | 0.13          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2  | 28       | 0.13          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3  | 28       | 0.13          |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1  | 28       | 0.13          |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2  | 28       | 0.13          |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3  | 28       | 0.13          |
| (3,1293) | 1:40:A:VAL:HG21 | 1:42:A:TRP:HE1  | 1        | 0.13          |
| (3,1293) | 1:40:A:VAL:HG22 | 1:42:A:TRP:HE1  | 1        | 0.13          |
| (3,1293) | 1:40:A:VAL:HG23 | 1:42:A:TRP:HE1  | 1        | 0.13          |
| (3,1293) | 1:40:A:VAL:HG21 | 1:42:A:TRP:HE1  | 37       | 0.13          |
| (3,1293) | 1:40:A:VAL:HG22 | 1:42:A:TRP:HE1  | 37       | 0.13          |
| (3,1293) | 1:40:A:VAL:HG23 | 1:42:A:TRP:HE1  | 37       | 0.13          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB | 28       | 0.13          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB | 28       | 0.13          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB | 28       | 0.13          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB | 29       | 0.13          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB | 29       | 0.13          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB | 29       | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 1        | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 2        | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 3        | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 4        | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 5        | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 6        | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 7        | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 8        | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 9        | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 10       | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 11       | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 12       | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 13       | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 14       | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 15       | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 17       | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 18       | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 19       | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 20       | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 21       | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 22       | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 23       | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 24       | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 25       | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 26       | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 27       | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 28       | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 29       | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 30       | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 31       | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 32       | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 34       | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 35       | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 36       | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 37       | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3 | 38       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3   | 39       | 0.13          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3   | 40       | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 1        | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 2        | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 3        | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 4        | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 5        | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 6        | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 7        | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 8        | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 9        | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 10       | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 11       | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 12       | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 13       | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 14       | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 15       | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 17       | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 18       | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 19       | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 20       | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 21       | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 22       | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 23       | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 24       | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 25       | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 26       | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 27       | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 28       | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 29       | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 30       | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 31       | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 32       | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 34       | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 35       | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 36       | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 37       | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 38       | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 39       | 0.13          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 40       | 0.13          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 21       | 0.13          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 21       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 21       | 0.13          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 21       | 0.13          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 21       | 0.13          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 21       | 0.13          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 21       | 0.13          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 21       | 0.13          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 21       | 0.13          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 24       | 0.13          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 24       | 0.13          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 24       | 0.13          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 24       | 0.13          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 24       | 0.13          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 24       | 0.13          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 24       | 0.13          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 24       | 0.13          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 24       | 0.13          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 29       | 0.13          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 29       | 0.13          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 29       | 0.13          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 29       | 0.13          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 29       | 0.13          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 29       | 0.13          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 29       | 0.13          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 29       | 0.13          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 29       | 0.13          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 32       | 0.13          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 32       | 0.13          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 32       | 0.13          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 32       | 0.13          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 32       | 0.13          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 32       | 0.13          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 32       | 0.13          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 32       | 0.13          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 32       | 0.13          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 35       | 0.13          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 35       | 0.13          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 35       | 0.13          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 35       | 0.13          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 35       | 0.13          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 35       | 0.13          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 35       | 0.13          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 35       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 35       | 0.13          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 37       | 0.13          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 37       | 0.13          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 37       | 0.13          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 37       | 0.13          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 37       | 0.13          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 37       | 0.13          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 37       | 0.13          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 37       | 0.13          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 37       | 0.13          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 38       | 0.13          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 38       | 0.13          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 38       | 0.13          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 38       | 0.13          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 38       | 0.13          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 38       | 0.13          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 38       | 0.13          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 38       | 0.13          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 38       | 0.13          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 39       | 0.13          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 39       | 0.13          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 39       | 0.13          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 39       | 0.13          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 39       | 0.13          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 39       | 0.13          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 39       | 0.13          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 39       | 0.13          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 39       | 0.13          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 16       | 0.13          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 16       | 0.13          |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 16       | 0.13          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 29       | 0.13          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 29       | 0.13          |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 29       | 0.13          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 40       | 0.13          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 40       | 0.13          |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 40       | 0.13          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 16       | 0.13          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 16       | 0.13          |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 16       | 0.13          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 29       | 0.13          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 29       | 0.13          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H  | 29       | 0.13          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H  | 40       | 0.13          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H  | 40       | 0.13          |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H  | 40       | 0.13          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA | 2        | 0.13          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA | 2        | 0.13          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA | 2        | 0.13          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA | 3        | 0.13          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA | 3        | 0.13          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA | 3        | 0.13          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA | 12       | 0.13          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA | 12       | 0.13          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA | 12       | 0.13          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA | 20       | 0.13          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA | 20       | 0.13          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA | 20       | 0.13          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA | 21       | 0.13          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA | 21       | 0.13          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA | 21       | 0.13          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA | 23       | 0.13          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA | 23       | 0.13          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA | 23       | 0.13          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA | 24       | 0.13          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA | 24       | 0.13          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA | 24       | 0.13          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA | 25       | 0.13          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA | 25       | 0.13          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA | 25       | 0.13          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA | 26       | 0.13          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA | 26       | 0.13          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA | 26       | 0.13          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA | 30       | 0.13          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA | 30       | 0.13          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA | 30       | 0.13          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA | 32       | 0.13          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA | 32       | 0.13          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA | 32       | 0.13          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA | 36       | 0.13          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA | 36       | 0.13          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA | 36       | 0.13          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA | 37       | 0.13          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA | 37       | 0.13          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA  | 37       | 0.13          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA  | 38       | 0.13          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA  | 38       | 0.13          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA  | 38       | 0.13          |
| (3,1261) | 1:67:A:THR:HG21 | 1:26:A:SER:HB2 | 25       | 0.13          |
| (3,1261) | 1:67:A:THR:HG22 | 1:26:A:SER:HB2 | 25       | 0.13          |
| (3,1261) | 1:67:A:THR:HG23 | 1:26:A:SER:HB2 | 25       | 0.13          |
| (3,1255) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3 | 20       | 0.13          |
| (3,1255) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3 | 20       | 0.13          |
| (3,1255) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3 | 20       | 0.13          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H   | 3        | 0.13          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H   | 3        | 0.13          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H   | 3        | 0.13          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H   | 8        | 0.13          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H   | 8        | 0.13          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H   | 8        | 0.13          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H   | 21       | 0.13          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H   | 21       | 0.13          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H   | 21       | 0.13          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H   | 28       | 0.13          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H   | 28       | 0.13          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H   | 28       | 0.13          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H   | 33       | 0.13          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H   | 33       | 0.13          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H   | 33       | 0.13          |
| (3,1243) | 1:13:A:THR:HG21 | 1:34:A:SER:H   | 16       | 0.13          |
| (3,1243) | 1:13:A:THR:HG22 | 1:34:A:SER:H   | 16       | 0.13          |
| (3,1243) | 1:13:A:THR:HG23 | 1:34:A:SER:H   | 16       | 0.13          |
| (3,1243) | 1:13:A:THR:HG21 | 1:34:A:SER:H   | 37       | 0.13          |
| (3,1243) | 1:13:A:THR:HG22 | 1:34:A:SER:H   | 37       | 0.13          |
| (3,1243) | 1:13:A:THR:HG23 | 1:34:A:SER:H   | 37       | 0.13          |
| (3,1243) | 1:13:A:THR:HG21 | 1:34:A:SER:H   | 38       | 0.13          |
| (3,1243) | 1:13:A:THR:HG22 | 1:34:A:SER:H   | 38       | 0.13          |
| (3,1243) | 1:13:A:THR:HG23 | 1:34:A:SER:H   | 38       | 0.13          |
| (3,1240) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3 | 5        | 0.13          |
| (3,1240) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3 | 5        | 0.13          |
| (3,1240) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3 | 5        | 0.13          |
| (3,1240) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3 | 10       | 0.13          |
| (3,1240) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3 | 10       | 0.13          |
| (3,1240) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3 | 10       | 0.13          |
| (3,1240) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3 | 13       | 0.13          |
| (3,1240) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3 | 13       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1240) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3  | 13       | 0.13          |
| (3,1240) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3  | 35       | 0.13          |
| (3,1240) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3  | 35       | 0.13          |
| (3,1240) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3  | 35       | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 3        | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 3        | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 3        | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 6        | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 6        | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 6        | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 8        | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 8        | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 8        | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 9        | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 9        | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 9        | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 10       | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 10       | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 10       | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 16       | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 16       | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 16       | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 19       | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 19       | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 19       | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 22       | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 22       | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 22       | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 26       | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 26       | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 26       | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 28       | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 28       | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 28       | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 40       | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 40       | 0.13          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 40       | 0.13          |
| (3,1221) | 1:69:A:HIS:H    | 1:56:A:ASN:H    | 3        | 0.13          |
| (3,1221) | 1:69:A:HIS:H    | 1:56:A:ASN:H    | 13       | 0.13          |
| (3,1221) | 1:69:A:HIS:H    | 1:56:A:ASN:H    | 16       | 0.13          |
| (3,1217) | 1:66:A:MET:H    | 1:28:A:THR:HA   | 16       | 0.13          |
| (3,1212) | 1:56:A:ASN:H    | 1:66:A:MET:HG2  | 23       | 0.13          |

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| Key      | Atom-1       | Atom-2         | Model ID | Violation (Å) |
|----------|--------------|----------------|----------|---------------|
| (3,1180) | 1:47:A:THR:H | 1:44:A:LYS:HB3 | 2        | 0.13          |
| (3,1180) | 1:47:A:THR:H | 1:44:A:LYS:HB3 | 31       | 0.13          |
| (3,1180) | 1:47:A:THR:H | 1:44:A:LYS:HB3 | 33       | 0.13          |
| (3,1180) | 1:47:A:THR:H | 1:44:A:LYS:HB3 | 38       | 0.13          |
| (3,1178) | 1:91:A:ALA:H | 1:84:A:ARG:HA  | 13       | 0.13          |
| (3,1167) | 1:75:A:ASP:H | 1:74:A:ASP:HB2 | 21       | 0.13          |
| (3,1167) | 1:75:A:ASP:H | 1:74:A:ASP:HB2 | 33       | 0.13          |
| (3,1126) | 1:78:A:VAL:H | 1:44:A:LYS:HE2 | 35       | 0.13          |
| (3,1096) | 1:74:A:ASP:H | 1:73:A:PRO:HA  | 25       | 0.13          |
| (3,1096) | 1:74:A:ASP:H | 1:73:A:PRO:HA  | 26       | 0.13          |
| (3,1096) | 1:74:A:ASP:H | 1:73:A:PRO:HA  | 28       | 0.13          |
| (3,1096) | 1:74:A:ASP:H | 1:73:A:PRO:HA  | 31       | 0.13          |
| (3,1096) | 1:74:A:ASP:H | 1:73:A:PRO:HA  | 34       | 0.13          |
| (3,1096) | 1:74:A:ASP:H | 1:73:A:PRO:HA  | 39       | 0.13          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 1        | 0.13          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 2        | 0.13          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 3        | 0.13          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 4        | 0.13          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 5        | 0.13          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 8        | 0.13          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 10       | 0.13          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 11       | 0.13          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 12       | 0.13          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 13       | 0.13          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 14       | 0.13          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 16       | 0.13          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 17       | 0.13          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 18       | 0.13          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 19       | 0.13          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 20       | 0.13          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 21       | 0.13          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 22       | 0.13          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 23       | 0.13          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 24       | 0.13          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 26       | 0.13          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 29       | 0.13          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 31       | 0.13          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 33       | 0.13          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 39       | 0.13          |
| (3,1085) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 40       | 0.13          |
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 1        | 0.13          |
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 2        | 0.13          |

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| Key      | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|----------|--------------|-----------------|----------|---------------|
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2  | 3        | 0.13          |
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2  | 4        | 0.13          |
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2  | 8        | 0.13          |
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2  | 12       | 0.13          |
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2  | 13       | 0.13          |
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2  | 19       | 0.13          |
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2  | 21       | 0.13          |
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2  | 22       | 0.13          |
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2  | 23       | 0.13          |
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2  | 24       | 0.13          |
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2  | 27       | 0.13          |
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2  | 30       | 0.13          |
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2  | 32       | 0.13          |
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2  | 33       | 0.13          |
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2  | 36       | 0.13          |
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2  | 37       | 0.13          |
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2  | 38       | 0.13          |
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2  | 39       | 0.13          |
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2  | 40       | 0.13          |
| (3,1019) | 1:48:A:GLU:H | 1:48:A:GLU:HG3  | 2        | 0.13          |
| (3,1019) | 1:48:A:GLU:H | 1:48:A:GLU:HG3  | 5        | 0.13          |
| (3,1019) | 1:48:A:GLU:H | 1:48:A:GLU:HG3  | 10       | 0.13          |
| (3,1019) | 1:48:A:GLU:H | 1:48:A:GLU:HG3  | 16       | 0.13          |
| (3,1019) | 1:48:A:GLU:H | 1:48:A:GLU:HG3  | 19       | 0.13          |
| (3,1019) | 1:48:A:GLU:H | 1:48:A:GLU:HG3  | 21       | 0.13          |
| (3,1019) | 1:48:A:GLU:H | 1:48:A:GLU:HG3  | 28       | 0.13          |
| (3,1019) | 1:48:A:GLU:H | 1:48:A:GLU:HG3  | 34       | 0.13          |
| (3,1019) | 1:48:A:GLU:H | 1:48:A:GLU:HG3  | 36       | 0.13          |
| (3,1003) | 1:5:A:PHE:H  | 1:4:A:PRO:HA    | 17       | 0.13          |
| (3,1003) | 1:5:A:PHE:H  | 1:4:A:PRO:HA    | 31       | 0.13          |
| (3,998)  | 1:79:A:TYR:H | 1:94:A:THR:HG21 | 1        | 0.13          |
| (3,998)  | 1:79:A:TYR:H | 1:94:A:THR:HG22 | 1        | 0.13          |
| (3,998)  | 1:79:A:TYR:H | 1:94:A:THR:HG23 | 1        | 0.13          |
| (3,998)  | 1:79:A:TYR:H | 1:94:A:THR:HG21 | 13       | 0.13          |
| (3,998)  | 1:79:A:TYR:H | 1:94:A:THR:HG22 | 13       | 0.13          |
| (3,998)  | 1:79:A:TYR:H | 1:94:A:THR:HG23 | 13       | 0.13          |
| (3,998)  | 1:79:A:TYR:H | 1:94:A:THR:HG21 | 36       | 0.13          |
| (3,998)  | 1:79:A:TYR:H | 1:94:A:THR:HG22 | 36       | 0.13          |
| (3,998)  | 1:79:A:TYR:H | 1:94:A:THR:HG23 | 36       | 0.13          |
| (3,998)  | 1:79:A:TYR:H | 1:94:A:THR:HG21 | 39       | 0.13          |
| (3,998)  | 1:79:A:TYR:H | 1:94:A:THR:HG22 | 39       | 0.13          |
| (3,998)  | 1:79:A:TYR:H | 1:94:A:THR:HG23 | 39       | 0.13          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,988) | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 20       | 0.13          |
| (3,988) | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 29       | 0.13          |
| (3,988) | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 33       | 0.13          |
| (3,988) | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 34       | 0.13          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 1        | 0.13          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 3        | 0.13          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 5        | 0.13          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 6        | 0.13          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 7        | 0.13          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 8        | 0.13          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 9        | 0.13          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 12       | 0.13          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 13       | 0.13          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 21       | 0.13          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 24       | 0.13          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 27       | 0.13          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 38       | 0.13          |
| (3,972) | 1:21:A:VAL:H | 1:21:A:VAL:HG21 | 9        | 0.13          |
| (3,972) | 1:21:A:VAL:H | 1:21:A:VAL:HG22 | 9        | 0.13          |
| (3,972) | 1:21:A:VAL:H | 1:21:A:VAL:HG23 | 9        | 0.13          |
| (3,972) | 1:21:A:VAL:H | 1:21:A:VAL:HG21 | 15       | 0.13          |
| (3,972) | 1:21:A:VAL:H | 1:21:A:VAL:HG22 | 15       | 0.13          |
| (3,972) | 1:21:A:VAL:H | 1:21:A:VAL:HG23 | 15       | 0.13          |
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 8        | 0.13          |
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 10       | 0.13          |
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 17       | 0.13          |
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 21       | 0.13          |
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 24       | 0.13          |
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 32       | 0.13          |
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 33       | 0.13          |
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 35       | 0.13          |
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 36       | 0.13          |
| (3,942) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 1        | 0.13          |
| (3,942) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 11       | 0.13          |
| (3,942) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 23       | 0.13          |
| (3,942) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 25       | 0.13          |
| (3,942) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 30       | 0.13          |
| (3,942) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 33       | 0.13          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 1        | 0.13          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 1        | 0.13          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 1        | 0.13          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 23       | 0.13          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 23       | 0.13          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 23       | 0.13          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 27       | 0.13          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 27       | 0.13          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 27       | 0.13          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 40       | 0.13          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 40       | 0.13          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 40       | 0.13          |
| (3,916) | 1:37:A:ASP:H | 1:37:A:ASP:HA   | 40       | 0.13          |
| (3,900) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 5        | 0.13          |
| (3,900) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 6        | 0.13          |
| (3,900) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 7        | 0.13          |
| (3,900) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 19       | 0.13          |
| (3,900) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 31       | 0.13          |
| (3,900) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 38       | 0.13          |
| (3,890) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 20       | 0.13          |
| (3,890) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 28       | 0.13          |
| (3,889) | 1:80:A:SER:H | 1:43:A:TYR:HB3  | 14       | 0.13          |
| (3,889) | 1:80:A:SER:H | 1:43:A:TYR:HB3  | 23       | 0.13          |
| (3,889) | 1:80:A:SER:H | 1:43:A:TYR:HB3  | 39       | 0.13          |
| (3,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3   | 16       | 0.13          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 21       | 0.13          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 21       | 0.13          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 21       | 0.13          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 24       | 0.13          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 24       | 0.13          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 24       | 0.13          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 25       | 0.13          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 25       | 0.13          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 25       | 0.13          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 28       | 0.13          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 28       | 0.13          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 28       | 0.13          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 29       | 0.13          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 29       | 0.13          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 29       | 0.13          |
| (3,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB   | 12       | 0.13          |
| (3,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB   | 16       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 3        | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 3        | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 3        | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 6        | 0.13          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 6        | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 6        | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 7        | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 7        | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 7        | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 8        | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 8        | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 8        | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 11       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 11       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 11       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 12       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 12       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 12       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 13       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 13       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 13       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 14       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 14       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 14       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 16       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 16       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 16       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 17       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 17       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 17       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 19       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 19       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 19       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 21       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 21       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 21       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 23       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 23       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 23       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 24       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 24       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 24       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 25       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 25       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 25       | 0.13          |
| (3,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 29       | 0.13          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG12 | 29       | 0.13          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG13 | 29       | 0.13          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG11 | 30       | 0.13          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG12 | 30       | 0.13          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG13 | 30       | 0.13          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG11 | 33       | 0.13          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG12 | 33       | 0.13          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG13 | 33       | 0.13          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG11 | 34       | 0.13          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG12 | 34       | 0.13          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG13 | 34       | 0.13          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG11 | 36       | 0.13          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG12 | 36       | 0.13          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG13 | 36       | 0.13          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG11 | 37       | 0.13          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG12 | 37       | 0.13          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG13 | 37       | 0.13          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG11 | 38       | 0.13          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG12 | 38       | 0.13          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG13 | 38       | 0.13          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG11 | 40       | 0.13          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG12 | 40       | 0.13          |
| (3,809) | 1:78:A:VAL:H  | 1:78:A:VAL:HG13 | 40       | 0.13          |
| (3,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 1        | 0.13          |
| (3,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 3        | 0.13          |
| (3,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 8        | 0.13          |
| (3,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 13       | 0.13          |
| (3,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 14       | 0.13          |
| (3,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 17       | 0.13          |
| (3,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 18       | 0.13          |
| (3,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 28       | 0.13          |
| (3,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 31       | 0.13          |
| (3,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 33       | 0.13          |
| (3,709) | 1:16:A:ILE:H  | 1:31:A:CYS:HB2  | 3        | 0.13          |
| (3,709) | 1:16:A:ILE:H  | 1:31:A:CYS:HB2  | 5        | 0.13          |
| (3,661) | 1:7:A:ALA:H   | 1:6:A:THR:HA    | 1        | 0.13          |
| (3,661) | 1:7:A:ALA:H   | 1:6:A:THR:HA    | 11       | 0.13          |
| (3,661) | 1:7:A:ALA:H   | 1:6:A:THR:HA    | 17       | 0.13          |
| (3,661) | 1:7:A:ALA:H   | 1:6:A:THR:HA    | 40       | 0.13          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 5        | 0.13          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 10       | 0.13          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 11       | 0.13          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 19       | 0.13          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 23       | 0.13          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 26       | 0.13          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 27       | 0.13          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 2        | 0.13          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 4        | 0.13          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 5        | 0.13          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 6        | 0.13          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 7        | 0.13          |
| (3,609) | 1:43:A:TYR:H  | 1:42:A:TRP:HB2  | 6        | 0.13          |
| (3,591) | 1:3:A:ASP:H   | 1:3:A:ASP:HA    | 16       | 0.13          |
| (3,589) | 1:93:A:SER:H  | 1:92:A:ARG:HG2  | 10       | 0.13          |
| (3,589) | 1:93:A:SER:H  | 1:92:A:ARG:HG2  | 16       | 0.13          |
| (3,589) | 1:93:A:SER:H  | 1:92:A:ARG:HG2  | 26       | 0.13          |
| (3,589) | 1:93:A:SER:H  | 1:92:A:ARG:HG2  | 36       | 0.13          |
| (3,589) | 1:93:A:SER:H  | 1:92:A:ARG:HG2  | 37       | 0.13          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 10       | 0.13          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 10       | 0.13          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 10       | 0.13          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 14       | 0.13          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 14       | 0.13          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 14       | 0.13          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 18       | 0.13          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 18       | 0.13          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 18       | 0.13          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 19       | 0.13          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 19       | 0.13          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 19       | 0.13          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 20       | 0.13          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 20       | 0.13          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 20       | 0.13          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 26       | 0.13          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 26       | 0.13          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 26       | 0.13          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 35       | 0.13          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 35       | 0.13          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 35       | 0.13          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 39       | 0.13          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 39       | 0.13          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 39       | 0.13          |
| (3,560) | 1:47:A:THR:H  | 1:47:A:THR:HA   | 5        | 0.13          |
| (3,558) | 1:47:A:THR:H  | 1:43:A:TYR:HD1  | 24       | 0.13          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2  | 24       | 0.13          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1  | 40       | 0.13          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2  | 40       | 0.13          |
| (3,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 3        | 0.13          |
| (3,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 6        | 0.13          |
| (3,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 9        | 0.13          |
| (3,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 11       | 0.13          |
| (3,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 14       | 0.13          |
| (3,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 15       | 0.13          |
| (3,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 19       | 0.13          |
| (3,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 21       | 0.13          |
| (3,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 22       | 0.13          |
| (3,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 28       | 0.13          |
| (3,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 7        | 0.13          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 6        | 0.13          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 2        | 0.13          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 10       | 0.13          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 18       | 0.13          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 20       | 0.13          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 22       | 0.13          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 38       | 0.13          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 4        | 0.13          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 10       | 0.13          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 15       | 0.13          |
| (3,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 16       | 0.13          |
| (3,419) | 1:69:A:HIS:H | 1:54:A:LYS:HA   | 6        | 0.13          |
| (3,419) | 1:69:A:HIS:H | 1:54:A:LYS:HA   | 18       | 0.13          |
| (3,410) | 1:96:A:GLU:H | 1:18:A:ASN:HD21 | 33       | 0.13          |
| (3,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD21 | 23       | 0.13          |
| (3,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD22 | 23       | 0.13          |
| (3,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD23 | 23       | 0.13          |
| (3,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD21 | 27       | 0.13          |
| (3,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD22 | 27       | 0.13          |
| (3,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD23 | 27       | 0.13          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 9        | 0.13          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 10       | 0.13          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 6        | 0.13          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 6        | 0.13          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 6        | 0.13          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 12       | 0.13          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 12       | 0.13          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 12       | 0.13          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 13       | 0.13          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 13       | 0.13          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 13       | 0.13          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 29       | 0.13          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 29       | 0.13          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 29       | 0.13          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 39       | 0.13          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 39       | 0.13          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 39       | 0.13          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 6        | 0.13          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 6        | 0.13          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 6        | 0.13          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 17       | 0.13          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 17       | 0.13          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 17       | 0.13          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 20       | 0.13          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 20       | 0.13          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 20       | 0.13          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 31       | 0.13          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 31       | 0.13          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 31       | 0.13          |
| (3,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 9        | 0.13          |
| (3,368) | 1:18:A:ASN:H | 1:17:A:GLN:HB3  | 28       | 0.13          |
| (3,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD1  | 3        | 0.13          |
| (3,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD2  | 3        | 0.13          |
| (3,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD1  | 4        | 0.13          |
| (3,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD2  | 4        | 0.13          |
| (3,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD1  | 36       | 0.13          |
| (3,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD2  | 36       | 0.13          |
| (3,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 2        | 0.13          |
| (3,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 18       | 0.13          |
| (3,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 19       | 0.13          |
| (3,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 33       | 0.13          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 16       | 0.13          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 16       | 0.13          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 16       | 0.13          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 29       | 0.13          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 29       | 0.13          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 29       | 0.13          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 40       | 0.13          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 40       | 0.13          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 40       | 0.13          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,239)  | 1:13:A:THR:H   | 1:14:A:LYS:HA  | 12       | 0.13          |
| (3,239)  | 1:13:A:THR:H   | 1:14:A:LYS:HA  | 13       | 0.13          |
| (3,239)  | 1:13:A:THR:H   | 1:14:A:LYS:HA  | 15       | 0.13          |
| (3,239)  | 1:13:A:THR:H   | 1:14:A:LYS:HA  | 22       | 0.13          |
| (3,239)  | 1:13:A:THR:H   | 1:14:A:LYS:HA  | 24       | 0.13          |
| (3,239)  | 1:13:A:THR:H   | 1:14:A:LYS:HA  | 28       | 0.13          |
| (3,239)  | 1:13:A:THR:H   | 1:14:A:LYS:HA  | 36       | 0.13          |
| (3,230)  | 1:13:A:THR:H   | 1:12:A:PHE:HD1 | 7        | 0.13          |
| (3,230)  | 1:13:A:THR:H   | 1:12:A:PHE:HD2 | 7        | 0.13          |
| (3,230)  | 1:13:A:THR:H   | 1:12:A:PHE:HD1 | 8        | 0.13          |
| (3,230)  | 1:13:A:THR:H   | 1:12:A:PHE:HD2 | 8        | 0.13          |
| (3,201)  | 1:90:A:GLU:H   | 1:89:A:GLY:HA2 | 7        | 0.13          |
| (3,201)  | 1:90:A:GLU:H   | 1:89:A:GLY:HA2 | 22       | 0.13          |
| (3,201)  | 1:90:A:GLU:H   | 1:89:A:GLY:HA2 | 23       | 0.13          |
| (3,201)  | 1:90:A:GLU:H   | 1:89:A:GLY:HA2 | 29       | 0.13          |
| (3,201)  | 1:90:A:GLU:H   | 1:89:A:GLY:HA2 | 31       | 0.13          |
| (3,201)  | 1:90:A:GLU:H   | 1:89:A:GLY:HA2 | 32       | 0.13          |
| (3,113)  | 1:63:A:CYS:H   | 1:60:A:ASP:H   | 19       | 0.13          |
| (3,50)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3 | 4        | 0.13          |
| (3,50)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3 | 6        | 0.13          |
| (3,50)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3 | 7        | 0.13          |
| (3,50)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3 | 17       | 0.13          |
| (3,50)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3 | 19       | 0.13          |
| (3,50)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3 | 28       | 0.13          |
| (3,50)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3 | 34       | 0.13          |
| (3,50)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3 | 35       | 0.13          |
| (3,50)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3 | 36       | 0.13          |
| (3,50)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3 | 39       | 0.13          |
| (3,39)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3 | 22       | 0.13          |
| (3,39)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3 | 23       | 0.13          |
| (3,39)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3 | 24       | 0.13          |
| (3,39)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3 | 28       | 0.13          |
| (3,39)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3 | 30       | 0.13          |
| (3,39)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3 | 34       | 0.13          |
| (3,39)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3 | 35       | 0.13          |
| (3,39)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3 | 36       | 0.13          |
| (3,39)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3 | 38       | 0.13          |
| (3,25)   | 1:89:A:GLY:H   | 1:88:A:ARG:HB3 | 8        | 0.13          |
| (1,3211) | 1:69:A:HIS:HE1 | 1:67:A:THR:HB  | 14       | 0.13          |
| (1,3211) | 1:69:A:HIS:HE1 | 1:67:A:THR:HB  | 21       | 0.13          |
| (1,3211) | 1:69:A:HIS:HE1 | 1:67:A:THR:HB  | 29       | 0.13          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1 | 2        | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 2        | 0.13          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 12       | 0.13          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 12       | 0.13          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 21       | 0.13          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 21       | 0.13          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 32       | 0.13          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 32       | 0.13          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 33       | 0.13          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 33       | 0.13          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 8        | 0.13          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 8        | 0.13          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 8        | 0.13          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 8        | 0.13          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 8        | 0.13          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 8        | 0.13          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 13       | 0.13          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 13       | 0.13          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 13       | 0.13          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 13       | 0.13          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 13       | 0.13          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 13       | 0.13          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 18       | 0.13          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 18       | 0.13          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 18       | 0.13          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 18       | 0.13          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 18       | 0.13          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 18       | 0.13          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 23       | 0.13          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 23       | 0.13          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 23       | 0.13          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 23       | 0.13          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 23       | 0.13          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 23       | 0.13          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 37       | 0.13          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 37       | 0.13          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 37       | 0.13          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 37       | 0.13          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 37       | 0.13          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 37       | 0.13          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 38       | 0.13          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 38       | 0.13          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 38       | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 38       | 0.13          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 38       | 0.13          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 38       | 0.13          |
| (1,3197) | 1:42:A:TRP:HZ2 | 1:30:A:GLU:HA   | 17       | 0.13          |
| (1,3197) | 1:42:A:TRP:HZ2 | 1:30:A:GLU:HA   | 27       | 0.13          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 2        | 0.13          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 2        | 0.13          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 2        | 0.13          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 2        | 0.13          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 15       | 0.13          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 15       | 0.13          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 15       | 0.13          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 15       | 0.13          |
| (1,3185) | 1:43:A:TYR:HD1 | 1:44:A:LYS:H    | 28       | 0.13          |
| (1,3185) | 1:43:A:TYR:HD2 | 1:44:A:LYS:H    | 28       | 0.13          |
| (1,3185) | 1:43:A:TYR:HD1 | 1:44:A:LYS:H    | 29       | 0.13          |
| (1,3185) | 1:43:A:TYR:HD2 | 1:44:A:LYS:H    | 29       | 0.13          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 6        | 0.13          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 6        | 0.13          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 6        | 0.13          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 8        | 0.13          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 8        | 0.13          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 8        | 0.13          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 12       | 0.13          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 12       | 0.13          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 12       | 0.13          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 13       | 0.13          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 13       | 0.13          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 13       | 0.13          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 40       | 0.13          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 40       | 0.13          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 40       | 0.13          |
| (1,3169) | 1:69:A:HIS:HD2 | 1:69:A:HIS:HB3  | 21       | 0.13          |
| (1,3169) | 1:69:A:HIS:HD2 | 1:69:A:HIS:HB3  | 22       | 0.13          |
| (1,3169) | 1:69:A:HIS:HD2 | 1:69:A:HIS:HB3  | 23       | 0.13          |
| (1,3169) | 1:69:A:HIS:HD2 | 1:69:A:HIS:HB3  | 24       | 0.13          |
| (1,3169) | 1:69:A:HIS:HD2 | 1:69:A:HIS:HB3  | 25       | 0.13          |
| (1,3169) | 1:69:A:HIS:HD2 | 1:69:A:HIS:HB3  | 30       | 0.13          |
| (1,3137) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3  | 3        | 0.13          |
| (1,3137) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 3        | 0.13          |
| (1,3137) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3  | 17       | 0.13          |
| (1,3137) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 17       | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3137) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3  | 29       | 0.13          |
| (1,3137) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 29       | 0.13          |
| (1,3137) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3  | 37       | 0.13          |
| (1,3137) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 37       | 0.13          |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2  | 31       | 0.13          |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2  | 31       | 0.13          |
| (1,3133) | 1:65:A:TYR:HE1 | 1:60:A:ASP:HB3  | 2        | 0.13          |
| (1,3133) | 1:65:A:TYR:HE2 | 1:60:A:ASP:HB3  | 2        | 0.13          |
| (1,3133) | 1:65:A:TYR:HE1 | 1:60:A:ASP:HB3  | 24       | 0.13          |
| (1,3133) | 1:65:A:TYR:HE2 | 1:60:A:ASP:HB3  | 24       | 0.13          |
| (1,3133) | 1:65:A:TYR:HE1 | 1:60:A:ASP:HB3  | 38       | 0.13          |
| (1,3133) | 1:65:A:TYR:HE2 | 1:60:A:ASP:HB3  | 38       | 0.13          |
| (1,3132) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB2  | 24       | 0.13          |
| (1,3132) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB2  | 24       | 0.13          |
| (1,3132) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB2  | 33       | 0.13          |
| (1,3132) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB2  | 33       | 0.13          |
| (1,3131) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3  | 4        | 0.13          |
| (1,3131) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3  | 4        | 0.13          |
| (1,3131) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3  | 11       | 0.13          |
| (1,3131) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3  | 11       | 0.13          |
| (1,3131) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3  | 35       | 0.13          |
| (1,3131) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3  | 35       | 0.13          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 6        | 0.13          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 6        | 0.13          |
| (1,3126) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 35       | 0.13          |
| (1,3126) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 35       | 0.13          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 6        | 0.13          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 6        | 0.13          |
| (1,3125) | 1:55:A:TYR:HD1 | 1:51:A:GLU:HA   | 35       | 0.13          |
| (1,3125) | 1:55:A:TYR:HD2 | 1:51:A:GLU:HA   | 35       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 7        | 0.13          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 7        | 0.13          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 7        | 0.13          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 7        | 0.13          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 7        | 0.13          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 7        | 0.13          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 10       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 10       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 10       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 10       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 10       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 10       | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 12       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 12       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 12       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 12       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 12       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 12       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 16       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 16       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 16       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 16       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 16       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 16       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 18       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 18       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 18       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 18       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 18       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 18       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 19       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 19       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 19       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 19       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 19       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 19       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 24       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 24       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 24       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 24       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 24       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 24       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 40       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 40       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 40       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 40       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 40       | 0.13          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 40       | 0.13          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 4        | 0.13          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 4        | 0.13          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 4        | 0.13          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 4        | 0.13          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 4        | 0.13          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 4        | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 22       | 0.13          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 22       | 0.13          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 22       | 0.13          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 22       | 0.13          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 22       | 0.13          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 22       | 0.13          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 31       | 0.13          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 31       | 0.13          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 31       | 0.13          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 31       | 0.13          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 31       | 0.13          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 31       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 3        | 0.13          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 3        | 0.13          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 3        | 0.13          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 3        | 0.13          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 9        | 0.13          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 9        | 0.13          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 9        | 0.13          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 9        | 0.13          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 10       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 10       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 10       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 10       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 12       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 12       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 12       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 12       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 14       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 14       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 14       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 14       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 21       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 21       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 21       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 21       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 23       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 23       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 23       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 23       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 27       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 27       | 0.13          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1 | 27       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2 | 27       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1 | 28       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2 | 28       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1 | 28       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2 | 28       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1 | 36       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2 | 36       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1 | 36       | 0.13          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2 | 36       | 0.13          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1 | 14       | 0.13          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2 | 14       | 0.13          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1 | 14       | 0.13          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2 | 14       | 0.13          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1 | 14       | 0.13          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2 | 14       | 0.13          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1 | 22       | 0.13          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2 | 22       | 0.13          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1 | 22       | 0.13          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2 | 22       | 0.13          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1 | 22       | 0.13          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2 | 22       | 0.13          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1 | 25       | 0.13          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2 | 25       | 0.13          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1 | 25       | 0.13          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2 | 25       | 0.13          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1 | 25       | 0.13          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2 | 25       | 0.13          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1 | 27       | 0.13          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2 | 27       | 0.13          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1 | 27       | 0.13          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2 | 27       | 0.13          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1 | 27       | 0.13          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2 | 27       | 0.13          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1 | 32       | 0.13          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2 | 32       | 0.13          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1 | 32       | 0.13          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2 | 32       | 0.13          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1 | 32       | 0.13          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2 | 32       | 0.13          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1 | 35       | 0.13          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2 | 35       | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 35       | 0.13          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 35       | 0.13          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 35       | 0.13          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 35       | 0.13          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 36       | 0.13          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 36       | 0.13          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 36       | 0.13          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 36       | 0.13          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 36       | 0.13          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 36       | 0.13          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 6        | 0.13          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 6        | 0.13          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 6        | 0.13          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 16       | 0.13          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 16       | 0.13          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 16       | 0.13          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 19       | 0.13          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 19       | 0.13          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 19       | 0.13          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 26       | 0.13          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 26       | 0.13          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 26       | 0.13          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 28       | 0.13          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 28       | 0.13          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 28       | 0.13          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 33       | 0.13          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 33       | 0.13          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 33       | 0.13          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 29       | 0.13          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 29       | 0.13          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 38       | 0.13          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 38       | 0.13          |
| (1,3033) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE1  | 14       | 0.13          |
| (1,3033) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE2  | 14       | 0.13          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 25       | 0.13          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 25       | 0.13          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 34       | 0.13          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 34       | 0.13          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 38       | 0.13          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 38       | 0.13          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 40       | 0.13          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 40       | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 13       | 0.13          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 13       | 0.13          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 13       | 0.13          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 18       | 0.13          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 18       | 0.13          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 18       | 0.13          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 25       | 0.13          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 25       | 0.13          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 25       | 0.13          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 27       | 0.13          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 27       | 0.13          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 27       | 0.13          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 30       | 0.13          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 30       | 0.13          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 30       | 0.13          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 34       | 0.13          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 34       | 0.13          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 34       | 0.13          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 36       | 0.13          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 36       | 0.13          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 36       | 0.13          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 37       | 0.13          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 37       | 0.13          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 37       | 0.13          |
| (1,3011) | 1:30:A:GLU:HB2 | 1:14:A:LYS:HE2  | 10       | 0.13          |
| (1,3011) | 1:30:A:GLU:HB2 | 1:14:A:LYS:HE2  | 21       | 0.13          |
| (1,3011) | 1:30:A:GLU:HB2 | 1:14:A:LYS:HE2  | 38       | 0.13          |
| (1,3011) | 1:30:A:GLU:HB2 | 1:14:A:LYS:HE2  | 39       | 0.13          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 6        | 0.13          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 6        | 0.13          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 6        | 0.13          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG21 | 39       | 0.13          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG22 | 39       | 0.13          |
| (1,3004) | 1:25:A:GLN:HB3 | 1:21:A:VAL:HG23 | 39       | 0.13          |
| (1,2974) | 1:65:A:TYR:HA  | 1:42:A:TRP:HZ2  | 3        | 0.13          |
| (1,2974) | 1:65:A:TYR:HA  | 1:42:A:TRP:HZ2  | 12       | 0.13          |
| (1,2974) | 1:65:A:TYR:HA  | 1:42:A:TRP:HZ2  | 19       | 0.13          |
| (1,2974) | 1:65:A:TYR:HA  | 1:42:A:TRP:HZ2  | 21       | 0.13          |
| (1,2974) | 1:65:A:TYR:HA  | 1:42:A:TRP:HZ2  | 24       | 0.13          |
| (1,2974) | 1:65:A:TYR:HA  | 1:42:A:TRP:HZ2  | 33       | 0.13          |
| (1,2967) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD2  | 2        | 0.13          |
| (1,2967) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD2  | 20       | 0.13          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 2        | 0.13          |
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 3        | 0.13          |
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 4        | 0.13          |
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 5        | 0.13          |
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 6        | 0.13          |
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 7        | 0.13          |
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 8        | 0.13          |
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 10       | 0.13          |
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 12       | 0.13          |
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 13       | 0.13          |
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 14       | 0.13          |
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 18       | 0.13          |
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 19       | 0.13          |
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 20       | 0.13          |
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 21       | 0.13          |
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 23       | 0.13          |
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 24       | 0.13          |
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 26       | 0.13          |
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 27       | 0.13          |
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 28       | 0.13          |
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 29       | 0.13          |
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 30       | 0.13          |
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 32       | 0.13          |
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 33       | 0.13          |
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 34       | 0.13          |
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 35       | 0.13          |
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 36       | 0.13          |
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 39       | 0.13          |
| (1,2953) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 40       | 0.13          |
| (1,2949) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 1        | 0.13          |
| (1,2949) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 4        | 0.13          |
| (1,2949) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 5        | 0.13          |
| (1,2949) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 7        | 0.13          |
| (1,2949) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 8        | 0.13          |
| (1,2949) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 10       | 0.13          |
| (1,2949) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 13       | 0.13          |
| (1,2949) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 14       | 0.13          |
| (1,2949) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 17       | 0.13          |
| (1,2949) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 21       | 0.13          |
| (1,2949) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 23       | 0.13          |
| (1,2949) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 28       | 0.13          |
| (1,2949) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 33       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2949) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 34       | 0.13          |
| (1,2949) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 37       | 0.13          |
| (1,2949) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 39       | 0.13          |
| (1,2937) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD1  | 3        | 0.13          |
| (1,2937) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD2  | 3        | 0.13          |
| (1,2937) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD1  | 17       | 0.13          |
| (1,2937) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD2  | 17       | 0.13          |
| (1,2937) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD1  | 29       | 0.13          |
| (1,2937) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD2  | 29       | 0.13          |
| (1,2937) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD1  | 37       | 0.13          |
| (1,2937) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD2  | 37       | 0.13          |
| (1,2931) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 4        | 0.13          |
| (1,2931) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 8        | 0.13          |
| (1,2931) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 31       | 0.13          |
| (1,2931) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 36       | 0.13          |
| (1,2929) | 1:17:A:GLN:HG2  | 1:17:A:GLN:H    | 28       | 0.13          |
| (1,2929) | 1:17:A:GLN:HG2  | 1:17:A:GLN:H    | 29       | 0.13          |
| (1,2903) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 4        | 0.13          |
| (1,2903) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 7        | 0.13          |
| (1,2903) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 10       | 0.13          |
| (1,2903) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 11       | 0.13          |
| (1,2903) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 12       | 0.13          |
| (1,2903) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 17       | 0.13          |
| (1,2903) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 21       | 0.13          |
| (1,2903) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 36       | 0.13          |
| (1,2903) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 38       | 0.13          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 7        | 0.13          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 20       | 0.13          |
| (1,2859) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 21       | 0.13          |
| (1,2859) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 24       | 0.13          |
| (1,2859) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 25       | 0.13          |
| (1,2859) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 28       | 0.13          |
| (1,2859) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 30       | 0.13          |
| (1,2859) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 32       | 0.13          |
| (1,2859) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 38       | 0.13          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 5        | 0.13          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 10       | 0.13          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 11       | 0.13          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 19       | 0.13          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 23       | 0.13          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 26       | 0.13          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 27       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 1        | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 3        | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 5        | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 7        | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 8        | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 9        | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 10       | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 12       | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 13       | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 14       | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 15       | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 16       | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 17       | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 18       | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 19       | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 20       | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 21       | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 22       | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 23       | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 24       | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 25       | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 26       | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 27       | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 28       | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 30       | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 32       | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 35       | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 36       | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 37       | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 38       | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 39       | 0.13          |
| (1,2767) | 1:100:A:GLU:HB2 | 1:100:A:GLU:HB3 | 40       | 0.13          |
| (1,2754) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 11       | 0.13          |
| (1,2754) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 14       | 0.13          |
| (1,2754) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 31       | 0.13          |
| (1,2745) | 1:86:A:GLU:HG2  | 1:86:A:GLU:H    | 12       | 0.13          |
| (1,2745) | 1:86:A:GLU:HG3  | 1:86:A:GLU:H    | 12       | 0.13          |
| (1,2745) | 1:86:A:GLU:HG2  | 1:86:A:GLU:H    | 28       | 0.13          |
| (1,2745) | 1:86:A:GLU:HG3  | 1:86:A:GLU:H    | 28       | 0.13          |
| (1,2723) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H    | 9        | 0.13          |
| (1,2713) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 7        | 0.13          |
| (1,2713) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 8        | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,2699) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA   | 4        | 0.13          |
| (1,2699) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA   | 14       | 0.13          |
| (1,2699) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA   | 33       | 0.13          |
| (1,2686) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 13       | 0.13          |
| (1,2686) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 14       | 0.13          |
| (1,2686) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 17       | 0.13          |
| (1,2686) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 21       | 0.13          |
| (1,2686) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 22       | 0.13          |
| (1,2686) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 24       | 0.13          |
| (1,2686) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 28       | 0.13          |
| (1,2686) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 35       | 0.13          |
| (1,2686) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 38       | 0.13          |
| (1,2686) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 39       | 0.13          |
| (1,2686) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 40       | 0.13          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 4        | 0.13          |
| (1,2675) | 1:25:A:GLN:HG3 | 1:26:A:SER:H    | 13       | 0.13          |
| (1,2675) | 1:25:A:GLN:HG3 | 1:26:A:SER:H    | 19       | 0.13          |
| (1,2675) | 1:25:A:GLN:HG3 | 1:26:A:SER:H    | 22       | 0.13          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 20       | 0.13          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 20       | 0.13          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 20       | 0.13          |
| (1,2649) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 9        | 0.13          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3   | 21       | 0.13          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3   | 24       | 0.13          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3   | 25       | 0.13          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3   | 36       | 0.13          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3   | 39       | 0.13          |
| (1,2550) | 1:92:A:ARG:HA  | 1:83:A:ALA:H    | 29       | 0.13          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA   | 2        | 0.13          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA   | 8        | 0.13          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA   | 12       | 0.13          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA   | 17       | 0.13          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA   | 20       | 0.13          |
| (1,2537) | 1:73:A:PRO:HG3 | 1:73:A:PRO:HA   | 27       | 0.13          |
| (1,2537) | 1:73:A:PRO:HG3 | 1:73:A:PRO:HA   | 29       | 0.13          |
| (1,2537) | 1:73:A:PRO:HG3 | 1:73:A:PRO:HA   | 34       | 0.13          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA    | 31       | 0.13          |
| (1,2487) | 1:9:A:PRO:HD2  | 1:9:A:PRO:HA    | 28       | 0.13          |
| (1,2479) | 1:9:A:PRO:HD2  | 1:8:A:GLU:HA    | 13       | 0.13          |
| (1,2479) | 1:9:A:PRO:HD2  | 1:8:A:GLU:HA    | 15       | 0.13          |
| (1,2460) | 1:4:A:PRO:HD3  | 1:3:A:ASP:HA    | 16       | 0.13          |
| (1,2460) | 1:4:A:PRO:HD3  | 1:3:A:ASP:HA    | 26       | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,2431) | 1:82:A:ILE:HB  | 1:41:A:THR:H    | 8        | 0.13          |
| (1,2431) | 1:82:A:ILE:HB  | 1:41:A:THR:H    | 32       | 0.13          |
| (1,2431) | 1:82:A:ILE:HB  | 1:41:A:THR:H    | 40       | 0.13          |
| (1,2416) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 6        | 0.13          |
| (1,2416) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 18       | 0.13          |
| (1,2416) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 20       | 0.13          |
| (1,2416) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 23       | 0.13          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2  | 22       | 0.13          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2  | 29       | 0.13          |
| (1,2402) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ   | 7        | 0.13          |
| (1,2402) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ   | 7        | 0.13          |
| (1,2402) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ   | 7        | 0.13          |
| (1,2402) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ   | 10       | 0.13          |
| (1,2402) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ   | 10       | 0.13          |
| (1,2402) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ   | 10       | 0.13          |
| (1,2402) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ   | 39       | 0.13          |
| (1,2402) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ   | 39       | 0.13          |
| (1,2402) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ   | 39       | 0.13          |
| (1,2339) | 1:26:A:SER:HB3 | 1:27:A:ALA:H    | 4        | 0.13          |
| (1,2339) | 1:26:A:SER:HB3 | 1:27:A:ALA:H    | 25       | 0.13          |
| (1,2331) | 1:26:A:SER:HA  | 1:68:A:ILE:HG21 | 31       | 0.13          |
| (1,2331) | 1:26:A:SER:HA  | 1:68:A:ILE:HG22 | 31       | 0.13          |
| (1,2331) | 1:26:A:SER:HA  | 1:68:A:ILE:HG23 | 31       | 0.13          |
| (1,2287) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H    | 2        | 0.13          |
| (1,2287) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H    | 3        | 0.13          |
| (1,2287) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H    | 6        | 0.13          |
| (1,2287) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H    | 9        | 0.13          |
| (1,2287) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H    | 14       | 0.13          |
| (1,2287) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H    | 19       | 0.13          |
| (1,2287) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H    | 25       | 0.13          |
| (1,2287) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H    | 31       | 0.13          |
| (1,2287) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H    | 33       | 0.13          |
| (1,2287) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H    | 35       | 0.13          |
| (1,2287) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H    | 37       | 0.13          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG21 | 2        | 0.13          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG22 | 2        | 0.13          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG23 | 2        | 0.13          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG21 | 17       | 0.13          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG22 | 17       | 0.13          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG23 | 17       | 0.13          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG21 | 21       | 0.13          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG22 | 21       | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG23 | 21       | 0.13          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG21 | 23       | 0.13          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG22 | 23       | 0.13          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG23 | 23       | 0.13          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG21 | 38       | 0.13          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG22 | 38       | 0.13          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG23 | 38       | 0.13          |
| (1,2250) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 27       | 0.13          |
| (1,2250) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 27       | 0.13          |
| (1,2237) | 1:18:A:ASN:HB2 | 1:18:A:ASN:H    | 6        | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 1        | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 2        | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 3        | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 4        | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 5        | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 6        | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 7        | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 8        | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 9        | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 10       | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 11       | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 12       | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 13       | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 14       | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 15       | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 17       | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 18       | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 19       | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 20       | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 21       | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 22       | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 23       | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 24       | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 25       | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 26       | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 27       | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 28       | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 29       | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 30       | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 31       | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 32       | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3  | 1:5:A:PHE:HB2   | 34       | 0.13          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2150) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2  | 35       | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2  | 36       | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2  | 37       | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2  | 38       | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2  | 39       | 0.13          |
| (1,2150) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2  | 40       | 0.13          |
| (1,2145) | 1:94:A:THR:HA   | 1:81:A:VAL:H   | 2        | 0.13          |
| (1,2145) | 1:94:A:THR:HA   | 1:81:A:VAL:H   | 30       | 0.13          |
| (1,2145) | 1:94:A:THR:HA   | 1:81:A:VAL:H   | 35       | 0.13          |
| (1,2145) | 1:94:A:THR:HA   | 1:81:A:VAL:H   | 38       | 0.13          |
| (1,2136) | 1:67:A:THR:HB   | 1:56:A:ASN:HB2 | 19       | 0.13          |
| (1,2099) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HA  | 37       | 0.13          |
| (1,2099) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HA  | 37       | 0.13          |
| (1,2099) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HA  | 37       | 0.13          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2 | 9        | 0.13          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2 | 9        | 0.13          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2 | 9        | 0.13          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2 | 20       | 0.13          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2 | 20       | 0.13          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2 | 20       | 0.13          |
| (1,2093) | 1:88:A:ARG:HD3  | 1:7:A:ALA:HA   | 23       | 0.13          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1 | 20       | 0.13          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2 | 20       | 0.13          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1 | 20       | 0.13          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2 | 20       | 0.13          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1 | 20       | 0.13          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2 | 20       | 0.13          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1 | 32       | 0.13          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2 | 32       | 0.13          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1 | 32       | 0.13          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2 | 32       | 0.13          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1 | 32       | 0.13          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2 | 32       | 0.13          |
| (1,2076) | 1:97:A:LEU:HD11 | 1:21:A:VAL:HB  | 7        | 0.13          |
| (1,2076) | 1:97:A:LEU:HD12 | 1:21:A:VAL:HB  | 7        | 0.13          |
| (1,2076) | 1:97:A:LEU:HD13 | 1:21:A:VAL:HB  | 7        | 0.13          |
| (1,2076) | 1:97:A:LEU:HD11 | 1:21:A:VAL:HB  | 34       | 0.13          |
| (1,2076) | 1:97:A:LEU:HD12 | 1:21:A:VAL:HB  | 34       | 0.13          |
| (1,2076) | 1:97:A:LEU:HD13 | 1:21:A:VAL:HB  | 34       | 0.13          |
| (1,2068) | 1:94:A:THR:HG21 | 1:93:A:SER:HA  | 17       | 0.13          |
| (1,2068) | 1:94:A:THR:HG22 | 1:93:A:SER:HA  | 17       | 0.13          |
| (1,2068) | 1:94:A:THR:HG23 | 1:93:A:SER:HA  | 17       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD11 | 1        | 0.13          |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD12 | 1        | 0.13          |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD13 | 1        | 0.13          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD11 | 1        | 0.13          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD12 | 1        | 0.13          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD13 | 1        | 0.13          |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD11 | 1        | 0.13          |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD12 | 1        | 0.13          |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD13 | 1        | 0.13          |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD11 | 10       | 0.13          |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD12 | 10       | 0.13          |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD13 | 10       | 0.13          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD11 | 10       | 0.13          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD12 | 10       | 0.13          |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD13 | 10       | 0.13          |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD11 | 10       | 0.13          |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD12 | 10       | 0.13          |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD13 | 10       | 0.13          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3  | 7        | 0.13          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3  | 7        | 0.13          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3  | 7        | 0.13          |
| (1,2064) | 1:85:A:LEU:HD11 | 1:88:A:ARG:HG3  | 18       | 0.13          |
| (1,2064) | 1:85:A:LEU:HD12 | 1:88:A:ARG:HG3  | 18       | 0.13          |
| (1,2064) | 1:85:A:LEU:HD13 | 1:88:A:ARG:HG3  | 18       | 0.13          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD21 | 34       | 0.13          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD22 | 34       | 0.13          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD23 | 34       | 0.13          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD21 | 34       | 0.13          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD22 | 34       | 0.13          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD23 | 34       | 0.13          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD21 | 34       | 0.13          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD22 | 34       | 0.13          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD23 | 34       | 0.13          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1  | 10       | 0.13          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2  | 10       | 0.13          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1  | 10       | 0.13          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2  | 10       | 0.13          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1  | 10       | 0.13          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2  | 10       | 0.13          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 20       | 0.13          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 20       | 0.13          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 20       | 0.13          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 1        | 0.13          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 1        | 0.13          |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 1        | 0.13          |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 12       | 0.13          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 12       | 0.13          |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 12       | 0.13          |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 30       | 0.13          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 30       | 0.13          |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 30       | 0.13          |
| (1,2014) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD1 | 35       | 0.13          |
| (1,2014) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD2 | 35       | 0.13          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1 | 18       | 0.13          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2 | 18       | 0.13          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3 | 18       | 0.13          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1 | 18       | 0.13          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2 | 18       | 0.13          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3 | 18       | 0.13          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1 | 18       | 0.13          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2 | 18       | 0.13          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3 | 18       | 0.13          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1 | 28       | 0.13          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2 | 28       | 0.13          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3 | 28       | 0.13          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1 | 28       | 0.13          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2 | 28       | 0.13          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3 | 28       | 0.13          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1 | 28       | 0.13          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2 | 28       | 0.13          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3 | 28       | 0.13          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 2        | 0.13          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 18       | 0.13          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 19       | 0.13          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 33       | 0.13          |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2 | 3        | 0.13          |
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2 | 3        | 0.13          |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2 | 3        | 0.13          |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2 | 15       | 0.13          |
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2 | 15       | 0.13          |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2 | 15       | 0.13          |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2 | 28       | 0.13          |
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2 | 28       | 0.13          |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2 | 28       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 29       | 0.13          |
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 29       | 0.13          |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 29       | 0.13          |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 39       | 0.13          |
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 39       | 0.13          |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 39       | 0.13          |
| (1,1994) | 1:21:A:VAL:HG11 | 1:25:A:GLN:HG3  | 27       | 0.13          |
| (1,1994) | 1:21:A:VAL:HG12 | 1:25:A:GLN:HG3  | 27       | 0.13          |
| (1,1994) | 1:21:A:VAL:HG13 | 1:25:A:GLN:HG3  | 27       | 0.13          |
| (1,1990) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 3        | 0.13          |
| (1,1990) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 3        | 0.13          |
| (1,1990) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 3        | 0.13          |
| (1,1990) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 11       | 0.13          |
| (1,1990) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 11       | 0.13          |
| (1,1990) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 11       | 0.13          |
| (1,1990) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 21       | 0.13          |
| (1,1990) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 21       | 0.13          |
| (1,1990) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 21       | 0.13          |
| (1,1990) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 23       | 0.13          |
| (1,1990) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 23       | 0.13          |
| (1,1990) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 23       | 0.13          |
| (1,1990) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 25       | 0.13          |
| (1,1990) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 25       | 0.13          |
| (1,1990) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 25       | 0.13          |
| (1,1990) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 26       | 0.13          |
| (1,1990) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 26       | 0.13          |
| (1,1990) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 26       | 0.13          |
| (1,1990) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 34       | 0.13          |
| (1,1990) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 34       | 0.13          |
| (1,1990) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 34       | 0.13          |
| (1,1990) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 36       | 0.13          |
| (1,1990) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 36       | 0.13          |
| (1,1990) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 36       | 0.13          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 11       | 0.13          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 29       | 0.13          |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H    | 7        | 0.13          |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H    | 7        | 0.13          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H    | 7        | 0.13          |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H    | 13       | 0.13          |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H    | 13       | 0.13          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H    | 13       | 0.13          |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H    | 20       | 0.13          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 20       | 0.13          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 20       | 0.13          |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 21       | 0.13          |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 21       | 0.13          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 21       | 0.13          |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 23       | 0.13          |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 23       | 0.13          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 23       | 0.13          |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 25       | 0.13          |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 25       | 0.13          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 25       | 0.13          |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 35       | 0.13          |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 35       | 0.13          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 35       | 0.13          |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 36       | 0.13          |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 36       | 0.13          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 36       | 0.13          |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 38       | 0.13          |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 38       | 0.13          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 38       | 0.13          |
| (1,1903) | 1:66:A:MET:HE1  | 1:79:A:TYR:HA  | 10       | 0.13          |
| (1,1903) | 1:66:A:MET:HE2  | 1:79:A:TYR:HA  | 10       | 0.13          |
| (1,1903) | 1:66:A:MET:HE3  | 1:79:A:TYR:HA  | 10       | 0.13          |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 3        | 0.13          |
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 3        | 0.13          |
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 3        | 0.13          |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 35       | 0.13          |
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 35       | 0.13          |
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 35       | 0.13          |
| (1,1896) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3 | 26       | 0.13          |
| (1,1896) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3 | 26       | 0.13          |
| (1,1896) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3 | 26       | 0.13          |
| (1,1861) | 1:7:A:ALA:HB1   | 1:88:A:ARG:HA  | 13       | 0.13          |
| (1,1861) | 1:7:A:ALA:HB2   | 1:88:A:ARG:HA  | 13       | 0.13          |
| (1,1861) | 1:7:A:ALA:HB3   | 1:88:A:ARG:HA  | 13       | 0.13          |
| (1,1861) | 1:7:A:ALA:HB1   | 1:88:A:ARG:HA  | 19       | 0.13          |
| (1,1861) | 1:7:A:ALA:HB2   | 1:88:A:ARG:HA  | 19       | 0.13          |
| (1,1861) | 1:7:A:ALA:HB3   | 1:88:A:ARG:HA  | 19       | 0.13          |
| (1,1861) | 1:7:A:ALA:HB1   | 1:88:A:ARG:HA  | 30       | 0.13          |
| (1,1861) | 1:7:A:ALA:HB2   | 1:88:A:ARG:HA  | 30       | 0.13          |
| (1,1861) | 1:7:A:ALA:HB3   | 1:88:A:ARG:HA  | 30       | 0.13          |
| (1,1853) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 6        | 0.13          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1853) | 1:27:A:ALA:HB2 | 1:28:A:THR:H   | 6        | 0.13          |
| (1,1853) | 1:27:A:ALA:HB3 | 1:28:A:THR:H   | 6        | 0.13          |
| (1,1853) | 1:27:A:ALA:HB1 | 1:28:A:THR:H   | 15       | 0.13          |
| (1,1853) | 1:27:A:ALA:HB2 | 1:28:A:THR:H   | 15       | 0.13          |
| (1,1853) | 1:27:A:ALA:HB3 | 1:28:A:THR:H   | 15       | 0.13          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2 | 2        | 0.13          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2 | 6        | 0.13          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2 | 8        | 0.13          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2 | 11       | 0.13          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2 | 16       | 0.13          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2 | 18       | 0.13          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2 | 26       | 0.13          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2 | 27       | 0.13          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2 | 28       | 0.13          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2 | 33       | 0.13          |
| (1,1811) | 1:98:A:LYS:HD2 | 1:98:A:LYS:HG2 | 37       | 0.13          |
| (1,1803) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3 | 2        | 0.13          |
| (1,1803) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3 | 3        | 0.13          |
| (1,1803) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3 | 4        | 0.13          |
| (1,1803) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3 | 5        | 0.13          |
| (1,1803) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3 | 6        | 0.13          |
| (1,1803) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3 | 7        | 0.13          |
| (1,1803) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3 | 8        | 0.13          |
| (1,1803) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3 | 10       | 0.13          |
| (1,1803) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3 | 12       | 0.13          |
| (1,1803) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3 | 13       | 0.13          |
| (1,1803) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3 | 14       | 0.13          |
| (1,1803) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3 | 18       | 0.13          |
| (1,1803) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3 | 19       | 0.13          |
| (1,1803) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3 | 20       | 0.13          |
| (1,1803) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3 | 21       | 0.13          |
| (1,1803) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3 | 23       | 0.13          |
| (1,1803) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3 | 24       | 0.13          |
| (1,1803) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3 | 26       | 0.13          |
| (1,1803) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3 | 27       | 0.13          |
| (1,1803) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3 | 28       | 0.13          |
| (1,1803) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3 | 29       | 0.13          |
| (1,1803) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3 | 30       | 0.13          |
| (1,1803) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3 | 32       | 0.13          |
| (1,1803) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3 | 33       | 0.13          |
| (1,1803) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3 | 34       | 0.13          |
| (1,1803) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3 | 35       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1803) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HB3  | 36       | 0.13          |
| (1,1803) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HB3  | 39       | 0.13          |
| (1,1803) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HB3  | 40       | 0.13          |
| (1,1725) | 1:38:A:ALA:HB1  | 1:83:A:ALA:HA   | 34       | 0.13          |
| (1,1725) | 1:38:A:ALA:HB2  | 1:83:A:ALA:HA   | 34       | 0.13          |
| (1,1725) | 1:38:A:ALA:HB3  | 1:83:A:ALA:HA   | 34       | 0.13          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG11 | 26       | 0.13          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG12 | 26       | 0.13          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG13 | 26       | 0.13          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG11 | 26       | 0.13          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG12 | 26       | 0.13          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 26       | 0.13          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 26       | 0.13          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 26       | 0.13          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 26       | 0.13          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG11 | 32       | 0.13          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG12 | 32       | 0.13          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG13 | 32       | 0.13          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG11 | 32       | 0.13          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG12 | 32       | 0.13          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 32       | 0.13          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 32       | 0.13          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 32       | 0.13          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 32       | 0.13          |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 9        | 0.13          |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 9        | 0.13          |
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 9        | 0.13          |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 11       | 0.13          |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 11       | 0.13          |
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 11       | 0.13          |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 16       | 0.13          |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 16       | 0.13          |
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 16       | 0.13          |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 17       | 0.13          |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 17       | 0.13          |
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 17       | 0.13          |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 18       | 0.13          |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 18       | 0.13          |
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 18       | 0.13          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 9        | 0.13          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 9        | 0.13          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 9        | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 9        | 0.13          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 9        | 0.13          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 9        | 0.13          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 9        | 0.13          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 9        | 0.13          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 9        | 0.13          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 31       | 0.13          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 31       | 0.13          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 31       | 0.13          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 31       | 0.13          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 31       | 0.13          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 31       | 0.13          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 31       | 0.13          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 31       | 0.13          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 31       | 0.13          |
| (1,1679) | 1:85:A:LEU:HD11 | 1:35:A:PHE:HD1  | 16       | 0.13          |
| (1,1679) | 1:85:A:LEU:HD11 | 1:35:A:PHE:HD2  | 16       | 0.13          |
| (1,1679) | 1:85:A:LEU:HD12 | 1:35:A:PHE:HD1  | 16       | 0.13          |
| (1,1679) | 1:85:A:LEU:HD12 | 1:35:A:PHE:HD2  | 16       | 0.13          |
| (1,1679) | 1:85:A:LEU:HD13 | 1:35:A:PHE:HD1  | 16       | 0.13          |
| (1,1679) | 1:85:A:LEU:HD13 | 1:35:A:PHE:HD2  | 16       | 0.13          |
| (1,1650) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 11       | 0.13          |
| (1,1650) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 11       | 0.13          |
| (1,1650) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 11       | 0.13          |
| (1,1650) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 11       | 0.13          |
| (1,1650) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 11       | 0.13          |
| (1,1650) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 11       | 0.13          |
| (1,1650) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 11       | 0.13          |
| (1,1650) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 11       | 0.13          |
| (1,1650) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 11       | 0.13          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 1        | 0.13          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 1        | 0.13          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 1        | 0.13          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 1        | 0.13          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 1        | 0.13          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 1        | 0.13          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 1        | 0.13          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 1        | 0.13          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 1        | 0.13          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 35       | 0.13          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 35       | 0.13          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 35       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 35       | 0.13          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 35       | 0.13          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 35       | 0.13          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 35       | 0.13          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 35       | 0.13          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 35       | 0.13          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 4        | 0.13          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 4        | 0.13          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 4        | 0.13          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 6        | 0.13          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 6        | 0.13          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 6        | 0.13          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 9        | 0.13          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 9        | 0.13          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 9        | 0.13          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 10       | 0.13          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 10       | 0.13          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 10       | 0.13          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 16       | 0.13          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 16       | 0.13          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 16       | 0.13          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 17       | 0.13          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 17       | 0.13          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 17       | 0.13          |
| (1,1624) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2  | 15       | 0.13          |
| (1,1624) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2  | 15       | 0.13          |
| (1,1624) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2  | 15       | 0.13          |
| (1,1624) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2  | 19       | 0.13          |
| (1,1624) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2  | 19       | 0.13          |
| (1,1624) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2  | 19       | 0.13          |
| (1,1623) | 1:82:A:ILE:HG21 | 1:84:A:ARG:HG2  | 6        | 0.13          |
| (1,1623) | 1:82:A:ILE:HG22 | 1:84:A:ARG:HG2  | 6        | 0.13          |
| (1,1623) | 1:82:A:ILE:HG23 | 1:84:A:ARG:HG2  | 6        | 0.13          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 2        | 0.13          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 2        | 0.13          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 2        | 0.13          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2  | 35       | 0.13          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2  | 35       | 0.13          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2  | 35       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1  | 7        | 0.13          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2  | 7        | 0.13          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1  | 7        | 0.13          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 7        | 0.13          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 7        | 0.13          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 7        | 0.13          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 10       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 10       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 10       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 10       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 10       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 10       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 12       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 12       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 12       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 12       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 12       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 12       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 16       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 16       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 16       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 16       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 16       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 16       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 18       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 18       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 18       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 18       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 18       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 18       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 19       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 19       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 19       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 19       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 19       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 19       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 24       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 24       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 24       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 24       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 24       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 24       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 40       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 40       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 40       | 0.13          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 40       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 40       | 0.13          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 40       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 8        | 0.13          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 8        | 0.13          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 8        | 0.13          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 8        | 0.13          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 8        | 0.13          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 8        | 0.13          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 12       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 12       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 12       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 12       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 12       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 12       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 18       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 18       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 18       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 18       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 18       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 18       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 21       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 21       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 21       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 21       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 21       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 21       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 23       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 23       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 23       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 23       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 23       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 23       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 33       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 33       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 33       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 33       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 33       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 33       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 40       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 40       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 40       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 40       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 40       | 0.13          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 40       | 0.13          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 15       | 0.13          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 15       | 0.13          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 15       | 0.13          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 18       | 0.13          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 18       | 0.13          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 18       | 0.13          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG21 | 24       | 0.13          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG22 | 24       | 0.13          |
| (1,1590) | 1:68:A:ILE:HB   | 1:71:A:VAL:HG23 | 24       | 0.13          |
| (1,1550) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA    | 23       | 0.13          |
| (1,1550) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA    | 23       | 0.13          |
| (1,1550) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA    | 23       | 0.13          |
| (1,1550) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA    | 31       | 0.13          |
| (1,1550) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA    | 31       | 0.13          |
| (1,1550) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA    | 31       | 0.13          |
| (1,1550) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA    | 40       | 0.13          |
| (1,1550) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA    | 40       | 0.13          |
| (1,1550) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA    | 40       | 0.13          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H    | 1        | 0.13          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H    | 1        | 0.13          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H    | 1        | 0.13          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H    | 8        | 0.13          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H    | 8        | 0.13          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H    | 8        | 0.13          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H    | 13       | 0.13          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H    | 13       | 0.13          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H    | 13       | 0.13          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H    | 14       | 0.13          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H    | 14       | 0.13          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H    | 14       | 0.13          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H    | 15       | 0.13          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H    | 15       | 0.13          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H    | 15       | 0.13          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H    | 21       | 0.13          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H    | 21       | 0.13          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H    | 21       | 0.13          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H    | 22       | 0.13          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H    | 22       | 0.13          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H    | 22       | 0.13          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H   | 27       | 0.13          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H   | 27       | 0.13          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H   | 27       | 0.13          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H   | 28       | 0.13          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H   | 28       | 0.13          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H   | 28       | 0.13          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H   | 35       | 0.13          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H   | 35       | 0.13          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H   | 35       | 0.13          |
| (1,1538) | 1:39:A:ILE:HG21 | 1:39:A:ILE:H   | 40       | 0.13          |
| (1,1538) | 1:39:A:ILE:HG22 | 1:39:A:ILE:H   | 40       | 0.13          |
| (1,1538) | 1:39:A:ILE:HG23 | 1:39:A:ILE:H   | 40       | 0.13          |
| (1,1514) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 10       | 0.13          |
| (1,1514) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 10       | 0.13          |
| (1,1514) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 10       | 0.13          |
| (1,1514) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 12       | 0.13          |
| (1,1514) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 12       | 0.13          |
| (1,1514) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 12       | 0.13          |
| (1,1514) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 21       | 0.13          |
| (1,1514) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 21       | 0.13          |
| (1,1514) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 21       | 0.13          |
| (1,1514) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 24       | 0.13          |
| (1,1514) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 24       | 0.13          |
| (1,1514) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 24       | 0.13          |
| (1,1514) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 27       | 0.13          |
| (1,1514) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 27       | 0.13          |
| (1,1514) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 27       | 0.13          |
| (1,1514) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 28       | 0.13          |
| (1,1514) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 28       | 0.13          |
| (1,1514) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 28       | 0.13          |
| (1,1513) | 1:66:A:MET:HE1  | 1:29:A:PHE:H   | 8        | 0.13          |
| (1,1513) | 1:66:A:MET:HE2  | 1:29:A:PHE:H   | 8        | 0.13          |
| (1,1513) | 1:66:A:MET:HE3  | 1:29:A:PHE:H   | 8        | 0.13          |
| (1,1513) | 1:66:A:MET:HE1  | 1:29:A:PHE:H   | 11       | 0.13          |
| (1,1513) | 1:66:A:MET:HE2  | 1:29:A:PHE:H   | 11       | 0.13          |
| (1,1513) | 1:66:A:MET:HE3  | 1:29:A:PHE:H   | 11       | 0.13          |
| (1,1513) | 1:66:A:MET:HE1  | 1:29:A:PHE:H   | 38       | 0.13          |
| (1,1513) | 1:66:A:MET:HE2  | 1:29:A:PHE:H   | 38       | 0.13          |
| (1,1513) | 1:66:A:MET:HE3  | 1:29:A:PHE:H   | 38       | 0.13          |
| (1,1510) | 1:66:A:MET:HE1  | 1:42:A:TRP:HE1 | 6        | 0.13          |
| (1,1510) | 1:66:A:MET:HE2  | 1:42:A:TRP:HE1 | 6        | 0.13          |
| (1,1510) | 1:66:A:MET:HE3  | 1:42:A:TRP:HE1 | 6        | 0.13          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1510) | 1:66:A:MET:HE1 | 1:42:A:TRP:HE1 | 8        | 0.13          |
| (1,1510) | 1:66:A:MET:HE2 | 1:42:A:TRP:HE1 | 8        | 0.13          |
| (1,1510) | 1:66:A:MET:HE3 | 1:42:A:TRP:HE1 | 8        | 0.13          |
| (1,1510) | 1:66:A:MET:HE1 | 1:42:A:TRP:HE1 | 12       | 0.13          |
| (1,1510) | 1:66:A:MET:HE2 | 1:42:A:TRP:HE1 | 12       | 0.13          |
| (1,1510) | 1:66:A:MET:HE3 | 1:42:A:TRP:HE1 | 12       | 0.13          |
| (1,1510) | 1:66:A:MET:HE1 | 1:42:A:TRP:HE1 | 13       | 0.13          |
| (1,1510) | 1:66:A:MET:HE2 | 1:42:A:TRP:HE1 | 13       | 0.13          |
| (1,1510) | 1:66:A:MET:HE3 | 1:42:A:TRP:HE1 | 13       | 0.13          |
| (1,1510) | 1:66:A:MET:HE1 | 1:42:A:TRP:HE1 | 40       | 0.13          |
| (1,1510) | 1:66:A:MET:HE2 | 1:42:A:TRP:HE1 | 40       | 0.13          |
| (1,1510) | 1:66:A:MET:HE3 | 1:42:A:TRP:HE1 | 40       | 0.13          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 2        | 0.13          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 2        | 0.13          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 2        | 0.13          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 2        | 0.13          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 2        | 0.13          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 2        | 0.13          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 10       | 0.13          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 10       | 0.13          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 10       | 0.13          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 10       | 0.13          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 10       | 0.13          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 10       | 0.13          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 18       | 0.13          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 18       | 0.13          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 18       | 0.13          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 18       | 0.13          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 18       | 0.13          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 18       | 0.13          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 24       | 0.13          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 24       | 0.13          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 24       | 0.13          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 24       | 0.13          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 24       | 0.13          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 24       | 0.13          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 28       | 0.13          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 28       | 0.13          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 28       | 0.13          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 28       | 0.13          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 28       | 0.13          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 28       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1508) | 1:66:A:MET:HE1  | 1:42:A:TRP:HZ3  | 4        | 0.13          |
| (1,1508) | 1:66:A:MET:HE2  | 1:42:A:TRP:HZ3  | 4        | 0.13          |
| (1,1508) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3  | 4        | 0.13          |
| (1,1508) | 1:66:A:MET:HE1  | 1:42:A:TRP:HZ3  | 14       | 0.13          |
| (1,1508) | 1:66:A:MET:HE2  | 1:42:A:TRP:HZ3  | 14       | 0.13          |
| (1,1508) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3  | 14       | 0.13          |
| (1,1508) | 1:66:A:MET:HE1  | 1:42:A:TRP:HZ3  | 17       | 0.13          |
| (1,1508) | 1:66:A:MET:HE2  | 1:42:A:TRP:HZ3  | 17       | 0.13          |
| (1,1508) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3  | 17       | 0.13          |
| (1,1507) | 1:66:A:MET:HE1  | 1:42:A:TRP:HB2  | 8        | 0.13          |
| (1,1507) | 1:66:A:MET:HE2  | 1:42:A:TRP:HB2  | 8        | 0.13          |
| (1,1507) | 1:66:A:MET:HE3  | 1:42:A:TRP:HB2  | 8        | 0.13          |
| (1,1507) | 1:66:A:MET:HE1  | 1:42:A:TRP:HB2  | 17       | 0.13          |
| (1,1507) | 1:66:A:MET:HE2  | 1:42:A:TRP:HB2  | 17       | 0.13          |
| (1,1507) | 1:66:A:MET:HE3  | 1:42:A:TRP:HB2  | 17       | 0.13          |
| (1,1507) | 1:66:A:MET:HE1  | 1:42:A:TRP:HB2  | 36       | 0.13          |
| (1,1507) | 1:66:A:MET:HE2  | 1:42:A:TRP:HB2  | 36       | 0.13          |
| (1,1507) | 1:66:A:MET:HE3  | 1:42:A:TRP:HB2  | 36       | 0.13          |
| (1,1502) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD11 | 3        | 0.13          |
| (1,1502) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD12 | 3        | 0.13          |
| (1,1502) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD13 | 3        | 0.13          |
| (1,1502) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD11 | 3        | 0.13          |
| (1,1502) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD12 | 3        | 0.13          |
| (1,1502) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD13 | 3        | 0.13          |
| (1,1502) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD11 | 3        | 0.13          |
| (1,1502) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD12 | 3        | 0.13          |
| (1,1502) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD13 | 3        | 0.13          |
| (1,1494) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 14       | 0.13          |
| (1,1494) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 14       | 0.13          |
| (1,1494) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 14       | 0.13          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA   | 14       | 0.13          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA   | 14       | 0.13          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA   | 14       | 0.13          |
| (1,1492) | 1:81:A:VAL:HG11 | 1:92:A:ARG:HA   | 18       | 0.13          |
| (1,1492) | 1:81:A:VAL:HG12 | 1:92:A:ARG:HA   | 18       | 0.13          |
| (1,1492) | 1:81:A:VAL:HG13 | 1:92:A:ARG:HA   | 18       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H    | 3        | 0.13          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H    | 3        | 0.13          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H    | 3        | 0.13          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H    | 6        | 0.13          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H    | 6        | 0.13          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H    | 6        | 0.13          |

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| Key      | Atom-1          | Atom-2       | Model ID | Violation (Å) |
|----------|-----------------|--------------|----------|---------------|
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 7        | 0.13          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 7        | 0.13          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 7        | 0.13          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 8        | 0.13          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 8        | 0.13          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 8        | 0.13          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 11       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 11       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 11       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 12       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 12       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 12       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 13       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 13       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 13       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 14       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 14       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 14       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 16       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 16       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 16       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 17       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 17       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 17       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 19       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 19       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 19       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 21       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 21       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 21       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 23       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 23       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 23       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 24       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 24       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 24       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 25       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 25       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 25       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H | 29       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H | 29       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H | 29       | 0.13          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H   | 30       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H   | 30       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H   | 30       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H   | 33       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H   | 33       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H   | 33       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H   | 34       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H   | 34       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H   | 34       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H   | 36       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H   | 36       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H   | 36       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H   | 37       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H   | 37       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H   | 37       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H   | 38       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H   | 38       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H   | 38       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG11 | 1:78:A:VAL:H   | 40       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG12 | 1:78:A:VAL:H   | 40       | 0.13          |
| (1,1476) | 1:78:A:VAL:HG13 | 1:78:A:VAL:H   | 40       | 0.13          |
| (1,1408) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HA | 5        | 0.13          |
| (1,1408) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HA | 5        | 0.13          |
| (1,1408) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HA | 5        | 0.13          |
| (1,1403) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H   | 6        | 0.13          |
| (1,1403) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H   | 6        | 0.13          |
| (1,1403) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H   | 6        | 0.13          |
| (1,1403) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H   | 17       | 0.13          |
| (1,1403) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H   | 17       | 0.13          |
| (1,1403) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H   | 17       | 0.13          |
| (1,1403) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H   | 20       | 0.13          |
| (1,1403) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H   | 20       | 0.13          |
| (1,1403) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H   | 20       | 0.13          |
| (1,1403) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H   | 31       | 0.13          |
| (1,1403) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H   | 31       | 0.13          |
| (1,1403) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H   | 31       | 0.13          |
| (1,1401) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H   | 3        | 0.13          |
| (1,1401) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H   | 3        | 0.13          |
| (1,1401) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H   | 3        | 0.13          |
| (1,1401) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H   | 13       | 0.13          |
| (1,1401) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H   | 13       | 0.13          |
| (1,1401) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H   | 13       | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1401) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H    | 19       | 0.13          |
| (1,1401) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H    | 19       | 0.13          |
| (1,1401) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 19       | 0.13          |
| (1,1401) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H    | 40       | 0.13          |
| (1,1401) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H    | 40       | 0.13          |
| (1,1401) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H    | 40       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 7        | 0.13          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 7        | 0.13          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 7        | 0.13          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 10       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 10       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 10       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 11       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 11       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 11       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 13       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 13       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 13       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 15       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 15       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 15       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 17       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 17       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 17       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 24       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 24       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 24       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 26       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 26       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 26       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 28       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 28       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 28       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 33       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 33       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 33       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 34       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 34       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 34       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB1 | 1:16:A:ILE:HG12 | 38       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB2 | 1:16:A:ILE:HG12 | 38       | 0.13          |
| (1,1400) | 1:95:A:ALA:HB3 | 1:16:A:ILE:HG12 | 38       | 0.13          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1387) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ  | 4        | 0.13          |
| (1,1387) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ  | 4        | 0.13          |
| (1,1387) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ  | 4        | 0.13          |
| (1,1387) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ  | 21       | 0.13          |
| (1,1387) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ  | 21       | 0.13          |
| (1,1387) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ  | 21       | 0.13          |
| (1,1387) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ  | 30       | 0.13          |
| (1,1387) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ  | 30       | 0.13          |
| (1,1387) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ  | 30       | 0.13          |
| (1,1387) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ  | 31       | 0.13          |
| (1,1387) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ  | 31       | 0.13          |
| (1,1387) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ  | 31       | 0.13          |
| (1,1387) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ  | 39       | 0.13          |
| (1,1387) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ  | 39       | 0.13          |
| (1,1387) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ  | 39       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 6        | 0.13          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 6        | 0.13          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 6        | 0.13          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 6        | 0.13          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 6        | 0.13          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 6        | 0.13          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 6        | 0.13          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 6        | 0.13          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 6        | 0.13          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 25       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 25       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 25       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 25       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 25       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 25       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 25       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 25       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 25       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 33       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 33       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 33       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 33       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 33       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 33       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 33       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 33       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 33       | 0.13          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 34       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 34       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 34       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 34       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 34       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 34       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 34       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 34       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 34       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 35       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 35       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 35       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 35       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 35       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 35       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 35       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 35       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 35       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 39       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 39       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 39       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 39       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 39       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 39       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 39       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 39       | 0.13          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 39       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 6        | 0.13          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 6        | 0.13          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 6        | 0.13          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 6        | 0.13          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 6        | 0.13          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 6        | 0.13          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 6        | 0.13          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 6        | 0.13          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 6        | 0.13          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 25       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 25       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 25       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 25       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 25       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 25       | 0.13          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 25       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 25       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 25       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 33       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 33       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 33       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 33       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 33       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 33       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 33       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 33       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 33       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 34       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 34       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 34       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 34       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 34       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 34       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 34       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 34       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 34       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 35       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 35       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 35       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 35       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 35       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 35       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 35       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 35       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 35       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 39       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 39       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 39       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 39       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 39       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 39       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 39       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 39       | 0.13          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 39       | 0.13          |
| (1,1368) | 1:16:A:ILE:HB  | 1:29:A:PHE:HB3 | 9        | 0.13          |
| (1,1368) | 1:16:A:ILE:HB  | 1:29:A:PHE:HB3 | 12       | 0.13          |
| (1,1368) | 1:16:A:ILE:HB  | 1:29:A:PHE:HB3 | 29       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 34       | 0.13          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 39       | 0.13          |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H    | 12       | 0.13          |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H    | 12       | 0.13          |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H    | 12       | 0.13          |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H    | 29       | 0.13          |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H    | 29       | 0.13          |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H    | 29       | 0.13          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA   | 1        | 0.13          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA   | 1        | 0.13          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA   | 1        | 0.13          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA   | 28       | 0.13          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA   | 28       | 0.13          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA   | 28       | 0.13          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 1        | 0.13          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 3        | 0.13          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 5        | 0.13          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 6        | 0.13          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 7        | 0.13          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 8        | 0.13          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 9        | 0.13          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 12       | 0.13          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 13       | 0.13          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 21       | 0.13          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 24       | 0.13          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 27       | 0.13          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 38       | 0.13          |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 4        | 0.13          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 28       | 0.13          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 28       | 0.13          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 28       | 0.13          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 29       | 0.13          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 29       | 0.13          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 29       | 0.13          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1  | 18       | 0.13          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2  | 18       | 0.13          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3  | 18       | 0.13          |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1  | 18       | 0.13          |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2  | 18       | 0.13          |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3  | 18       | 0.13          |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1  | 18       | 0.13          |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2  | 18       | 0.13          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3 | 18       | 0.13          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1 | 28       | 0.13          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2 | 28       | 0.13          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3 | 28       | 0.13          |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1 | 28       | 0.13          |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2 | 28       | 0.13          |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3 | 28       | 0.13          |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1 | 28       | 0.13          |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2 | 28       | 0.13          |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3 | 28       | 0.13          |
| (1,1289) | 1:40:A:VAL:HG21 | 1:42:A:TRP:HE1 | 1        | 0.13          |
| (1,1289) | 1:40:A:VAL:HG22 | 1:42:A:TRP:HE1 | 1        | 0.13          |
| (1,1289) | 1:40:A:VAL:HG23 | 1:42:A:TRP:HE1 | 1        | 0.13          |
| (1,1289) | 1:40:A:VAL:HG21 | 1:42:A:TRP:HE1 | 37       | 0.13          |
| (1,1289) | 1:40:A:VAL:HG22 | 1:42:A:TRP:HE1 | 37       | 0.13          |
| (1,1289) | 1:40:A:VAL:HG23 | 1:42:A:TRP:HE1 | 37       | 0.13          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB  | 28       | 0.13          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB  | 28       | 0.13          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB  | 28       | 0.13          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB  | 29       | 0.13          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB  | 29       | 0.13          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB  | 29       | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3  | 1        | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3  | 2        | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3  | 3        | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3  | 4        | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3  | 5        | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3  | 6        | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3  | 7        | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3  | 8        | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3  | 9        | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3  | 10       | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3  | 11       | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3  | 12       | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3  | 13       | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3  | 14       | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3  | 15       | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3  | 17       | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3  | 18       | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3  | 19       | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3  | 20       | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3  | 21       | 0.13          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,1270) | 1:5:A:PHE:HB2 | 1:5:A:PHE:HB3 | 22       | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2 | 1:5:A:PHE:HB3 | 23       | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2 | 1:5:A:PHE:HB3 | 24       | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2 | 1:5:A:PHE:HB3 | 25       | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2 | 1:5:A:PHE:HB3 | 26       | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2 | 1:5:A:PHE:HB3 | 27       | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2 | 1:5:A:PHE:HB3 | 28       | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2 | 1:5:A:PHE:HB3 | 29       | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2 | 1:5:A:PHE:HB3 | 30       | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2 | 1:5:A:PHE:HB3 | 31       | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2 | 1:5:A:PHE:HB3 | 32       | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2 | 1:5:A:PHE:HB3 | 34       | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2 | 1:5:A:PHE:HB3 | 35       | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2 | 1:5:A:PHE:HB3 | 36       | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2 | 1:5:A:PHE:HB3 | 37       | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2 | 1:5:A:PHE:HB3 | 38       | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2 | 1:5:A:PHE:HB3 | 39       | 0.13          |
| (1,1270) | 1:5:A:PHE:HB2 | 1:5:A:PHE:HB3 | 40       | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3 | 1:5:A:PHE:HB2 | 1        | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3 | 1:5:A:PHE:HB2 | 2        | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3 | 1:5:A:PHE:HB2 | 3        | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3 | 1:5:A:PHE:HB2 | 4        | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3 | 1:5:A:PHE:HB2 | 5        | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3 | 1:5:A:PHE:HB2 | 6        | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3 | 1:5:A:PHE:HB2 | 7        | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3 | 1:5:A:PHE:HB2 | 8        | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3 | 1:5:A:PHE:HB2 | 9        | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3 | 1:5:A:PHE:HB2 | 10       | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3 | 1:5:A:PHE:HB2 | 11       | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3 | 1:5:A:PHE:HB2 | 12       | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3 | 1:5:A:PHE:HB2 | 13       | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3 | 1:5:A:PHE:HB2 | 14       | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3 | 1:5:A:PHE:HB2 | 15       | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3 | 1:5:A:PHE:HB2 | 17       | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3 | 1:5:A:PHE:HB2 | 18       | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3 | 1:5:A:PHE:HB2 | 19       | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3 | 1:5:A:PHE:HB2 | 20       | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3 | 1:5:A:PHE:HB2 | 21       | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3 | 1:5:A:PHE:HB2 | 22       | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3 | 1:5:A:PHE:HB2 | 23       | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3 | 1:5:A:PHE:HB2 | 24       | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3 | 1:5:A:PHE:HB2 | 25       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1269) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 26       | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 27       | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 28       | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 29       | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 30       | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 31       | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 32       | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 34       | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 35       | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 36       | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 37       | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 38       | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 39       | 0.13          |
| (1,1269) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 40       | 0.13          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 21       | 0.13          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 21       | 0.13          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 21       | 0.13          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 21       | 0.13          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 21       | 0.13          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 21       | 0.13          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 21       | 0.13          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 21       | 0.13          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 21       | 0.13          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 24       | 0.13          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 24       | 0.13          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 24       | 0.13          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 24       | 0.13          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 24       | 0.13          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 24       | 0.13          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 24       | 0.13          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 24       | 0.13          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 24       | 0.13          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 29       | 0.13          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 29       | 0.13          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 29       | 0.13          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 29       | 0.13          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 29       | 0.13          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 29       | 0.13          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 29       | 0.13          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 29       | 0.13          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 29       | 0.13          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 32       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 32       | 0.13          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 32       | 0.13          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 32       | 0.13          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 32       | 0.13          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 32       | 0.13          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 32       | 0.13          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 32       | 0.13          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 32       | 0.13          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 35       | 0.13          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 35       | 0.13          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 35       | 0.13          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 35       | 0.13          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 35       | 0.13          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 35       | 0.13          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 35       | 0.13          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 35       | 0.13          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 35       | 0.13          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 37       | 0.13          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 37       | 0.13          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 37       | 0.13          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 37       | 0.13          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 37       | 0.13          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 37       | 0.13          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 37       | 0.13          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 37       | 0.13          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 37       | 0.13          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 38       | 0.13          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 38       | 0.13          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 38       | 0.13          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 38       | 0.13          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 38       | 0.13          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 38       | 0.13          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 38       | 0.13          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 38       | 0.13          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 38       | 0.13          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 39       | 0.13          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 39       | 0.13          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 39       | 0.13          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 39       | 0.13          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 39       | 0.13          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 39       | 0.13          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 39       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 39       | 0.13          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 39       | 0.13          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 16       | 0.13          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 16       | 0.13          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 16       | 0.13          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 29       | 0.13          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 29       | 0.13          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 29       | 0.13          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 40       | 0.13          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 40       | 0.13          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 40       | 0.13          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 16       | 0.13          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 16       | 0.13          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 16       | 0.13          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 29       | 0.13          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 29       | 0.13          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 29       | 0.13          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 40       | 0.13          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 40       | 0.13          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 40       | 0.13          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 2        | 0.13          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 2        | 0.13          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 2        | 0.13          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 3        | 0.13          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 3        | 0.13          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 3        | 0.13          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 12       | 0.13          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 12       | 0.13          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 12       | 0.13          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 20       | 0.13          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 20       | 0.13          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 20       | 0.13          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 21       | 0.13          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 21       | 0.13          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 21       | 0.13          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 23       | 0.13          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 23       | 0.13          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 23       | 0.13          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 24       | 0.13          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 24       | 0.13          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 24       | 0.13          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 25       | 0.13          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA  | 25       | 0.13          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA  | 25       | 0.13          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA  | 26       | 0.13          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA  | 26       | 0.13          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA  | 26       | 0.13          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA  | 30       | 0.13          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA  | 30       | 0.13          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA  | 30       | 0.13          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA  | 32       | 0.13          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA  | 32       | 0.13          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA  | 32       | 0.13          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA  | 36       | 0.13          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA  | 36       | 0.13          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA  | 36       | 0.13          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA  | 37       | 0.13          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA  | 37       | 0.13          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA  | 37       | 0.13          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA  | 38       | 0.13          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA  | 38       | 0.13          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA  | 38       | 0.13          |
| (1,1257) | 1:67:A:THR:HG21 | 1:26:A:SER:HB2 | 25       | 0.13          |
| (1,1257) | 1:67:A:THR:HG22 | 1:26:A:SER:HB2 | 25       | 0.13          |
| (1,1257) | 1:67:A:THR:HG23 | 1:26:A:SER:HB2 | 25       | 0.13          |
| (1,1251) | 1:41:A:THR:HG21 | 1:48:A:GLU:HB3 | 20       | 0.13          |
| (1,1251) | 1:41:A:THR:HG22 | 1:48:A:GLU:HB3 | 20       | 0.13          |
| (1,1251) | 1:41:A:THR:HG23 | 1:48:A:GLU:HB3 | 20       | 0.13          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H   | 3        | 0.13          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H   | 3        | 0.13          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H   | 3        | 0.13          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H   | 8        | 0.13          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H   | 8        | 0.13          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H   | 8        | 0.13          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H   | 21       | 0.13          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H   | 21       | 0.13          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H   | 21       | 0.13          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H   | 28       | 0.13          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H   | 28       | 0.13          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H   | 28       | 0.13          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H   | 33       | 0.13          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H   | 33       | 0.13          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H   | 33       | 0.13          |
| (1,1239) | 1:13:A:THR:HG21 | 1:34:A:SER:H   | 16       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1239) | 1:13:A:THR:HG22 | 1:34:A:SER:H    | 16       | 0.13          |
| (1,1239) | 1:13:A:THR:HG23 | 1:34:A:SER:H    | 16       | 0.13          |
| (1,1239) | 1:13:A:THR:HG21 | 1:34:A:SER:H    | 37       | 0.13          |
| (1,1239) | 1:13:A:THR:HG22 | 1:34:A:SER:H    | 37       | 0.13          |
| (1,1239) | 1:13:A:THR:HG23 | 1:34:A:SER:H    | 37       | 0.13          |
| (1,1239) | 1:13:A:THR:HG21 | 1:34:A:SER:H    | 38       | 0.13          |
| (1,1239) | 1:13:A:THR:HG22 | 1:34:A:SER:H    | 38       | 0.13          |
| (1,1239) | 1:13:A:THR:HG23 | 1:34:A:SER:H    | 38       | 0.13          |
| (1,1236) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3  | 5        | 0.13          |
| (1,1236) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3  | 5        | 0.13          |
| (1,1236) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3  | 5        | 0.13          |
| (1,1236) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3  | 10       | 0.13          |
| (1,1236) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3  | 10       | 0.13          |
| (1,1236) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3  | 10       | 0.13          |
| (1,1236) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3  | 13       | 0.13          |
| (1,1236) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3  | 13       | 0.13          |
| (1,1236) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3  | 13       | 0.13          |
| (1,1236) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3  | 35       | 0.13          |
| (1,1236) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3  | 35       | 0.13          |
| (1,1236) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3  | 35       | 0.13          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 3        | 0.13          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 3        | 0.13          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 3        | 0.13          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 6        | 0.13          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 6        | 0.13          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 6        | 0.13          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 8        | 0.13          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 8        | 0.13          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 8        | 0.13          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 9        | 0.13          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 9        | 0.13          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 9        | 0.13          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 10       | 0.13          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 10       | 0.13          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 10       | 0.13          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 16       | 0.13          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 16       | 0.13          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 16       | 0.13          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 19       | 0.13          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 19       | 0.13          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 19       | 0.13          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 22       | 0.13          |

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| Key      | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|----------|--------------|-----------------|----------|---------------|
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD22 | 22       | 0.13          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD23 | 22       | 0.13          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD21 | 26       | 0.13          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD22 | 26       | 0.13          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD23 | 26       | 0.13          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD21 | 28       | 0.13          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD22 | 28       | 0.13          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD23 | 28       | 0.13          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD21 | 40       | 0.13          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD22 | 40       | 0.13          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD23 | 40       | 0.13          |
| (1,1217) | 1:69:A:HIS:H | 1:56:A:ASN:H    | 3        | 0.13          |
| (1,1217) | 1:69:A:HIS:H | 1:56:A:ASN:H    | 13       | 0.13          |
| (1,1217) | 1:69:A:HIS:H | 1:56:A:ASN:H    | 16       | 0.13          |
| (1,1213) | 1:66:A:MET:H | 1:28:A:THR:HA   | 16       | 0.13          |
| (1,1208) | 1:56:A:ASN:H | 1:66:A:MET:HG2  | 23       | 0.13          |
| (1,1176) | 1:47:A:THR:H | 1:44:A:LYS:HB3  | 2        | 0.13          |
| (1,1176) | 1:47:A:THR:H | 1:44:A:LYS:HB3  | 31       | 0.13          |
| (1,1176) | 1:47:A:THR:H | 1:44:A:LYS:HB3  | 33       | 0.13          |
| (1,1176) | 1:47:A:THR:H | 1:44:A:LYS:HB3  | 38       | 0.13          |
| (1,1174) | 1:91:A:ALA:H | 1:84:A:ARG:HA   | 13       | 0.13          |
| (1,1163) | 1:75:A:ASP:H | 1:74:A:ASP:HB2  | 21       | 0.13          |
| (1,1163) | 1:75:A:ASP:H | 1:74:A:ASP:HB2  | 33       | 0.13          |
| (1,1125) | 1:78:A:VAL:H | 1:44:A:LYS:HE2  | 35       | 0.13          |
| (1,1095) | 1:74:A:ASP:H | 1:73:A:PRO:HA   | 25       | 0.13          |
| (1,1095) | 1:74:A:ASP:H | 1:73:A:PRO:HA   | 26       | 0.13          |
| (1,1095) | 1:74:A:ASP:H | 1:73:A:PRO:HA   | 28       | 0.13          |
| (1,1095) | 1:74:A:ASP:H | 1:73:A:PRO:HA   | 31       | 0.13          |
| (1,1095) | 1:74:A:ASP:H | 1:73:A:PRO:HA   | 34       | 0.13          |
| (1,1095) | 1:74:A:ASP:H | 1:73:A:PRO:HA   | 39       | 0.13          |
| (1,1084) | 1:99:A:GLY:H | 1:99:A:GLY:HA2  | 1        | 0.13          |
| (1,1084) | 1:99:A:GLY:H | 1:99:A:GLY:HA2  | 2        | 0.13          |
| (1,1084) | 1:99:A:GLY:H | 1:99:A:GLY:HA2  | 3        | 0.13          |
| (1,1084) | 1:99:A:GLY:H | 1:99:A:GLY:HA2  | 4        | 0.13          |
| (1,1084) | 1:99:A:GLY:H | 1:99:A:GLY:HA2  | 5        | 0.13          |
| (1,1084) | 1:99:A:GLY:H | 1:99:A:GLY:HA2  | 8        | 0.13          |
| (1,1084) | 1:99:A:GLY:H | 1:99:A:GLY:HA2  | 10       | 0.13          |
| (1,1084) | 1:99:A:GLY:H | 1:99:A:GLY:HA2  | 11       | 0.13          |
| (1,1084) | 1:99:A:GLY:H | 1:99:A:GLY:HA2  | 12       | 0.13          |
| (1,1084) | 1:99:A:GLY:H | 1:99:A:GLY:HA2  | 13       | 0.13          |
| (1,1084) | 1:99:A:GLY:H | 1:99:A:GLY:HA2  | 14       | 0.13          |
| (1,1084) | 1:99:A:GLY:H | 1:99:A:GLY:HA2  | 16       | 0.13          |

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| Key      | Atom-1       | Atom-2         | Model ID | Violation (Å) |
|----------|--------------|----------------|----------|---------------|
| (1,1084) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 17       | 0.13          |
| (1,1084) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 18       | 0.13          |
| (1,1084) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 19       | 0.13          |
| (1,1084) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 20       | 0.13          |
| (1,1084) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 21       | 0.13          |
| (1,1084) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 22       | 0.13          |
| (1,1084) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 23       | 0.13          |
| (1,1084) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 24       | 0.13          |
| (1,1084) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 26       | 0.13          |
| (1,1084) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 29       | 0.13          |
| (1,1084) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 31       | 0.13          |
| (1,1084) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 33       | 0.13          |
| (1,1084) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 39       | 0.13          |
| (1,1084) | 1:99:A:GLY:H | 1:99:A:GLY:HA2 | 40       | 0.13          |
| (1,1052) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 1        | 0.13          |
| (1,1052) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 2        | 0.13          |
| (1,1052) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 3        | 0.13          |
| (1,1052) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 4        | 0.13          |
| (1,1052) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 8        | 0.13          |
| (1,1052) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 12       | 0.13          |
| (1,1052) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 13       | 0.13          |
| (1,1052) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 19       | 0.13          |
| (1,1052) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 21       | 0.13          |
| (1,1052) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 22       | 0.13          |
| (1,1052) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 23       | 0.13          |
| (1,1052) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 24       | 0.13          |
| (1,1052) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 27       | 0.13          |
| (1,1052) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 30       | 0.13          |
| (1,1052) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 32       | 0.13          |
| (1,1052) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 33       | 0.13          |
| (1,1052) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 36       | 0.13          |
| (1,1052) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 37       | 0.13          |
| (1,1052) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 38       | 0.13          |
| (1,1052) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 39       | 0.13          |
| (1,1052) | 1:26:A:SER:H | 1:25:A:GLN:HG2 | 40       | 0.13          |
| (1,1020) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 2        | 0.13          |
| (1,1020) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 5        | 0.13          |
| (1,1020) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 10       | 0.13          |
| (1,1020) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 16       | 0.13          |
| (1,1020) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 19       | 0.13          |
| (1,1020) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 21       | 0.13          |
| (1,1020) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 28       | 0.13          |

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| Key      | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|----------|--------------|-----------------|----------|---------------|
| (1,1020) | 1:48:A:GLU:H | 1:48:A:GLU:HG3  | 34       | 0.13          |
| (1,1020) | 1:48:A:GLU:H | 1:48:A:GLU:HG3  | 36       | 0.13          |
| (1,1002) | 1:5:A:PHE:H  | 1:4:A:PRO:HA    | 17       | 0.13          |
| (1,1002) | 1:5:A:PHE:H  | 1:4:A:PRO:HA    | 31       | 0.13          |
| (1,997)  | 1:79:A:TYR:H | 1:94:A:THR:HG21 | 1        | 0.13          |
| (1,997)  | 1:79:A:TYR:H | 1:94:A:THR:HG22 | 1        | 0.13          |
| (1,997)  | 1:79:A:TYR:H | 1:94:A:THR:HG23 | 1        | 0.13          |
| (1,997)  | 1:79:A:TYR:H | 1:94:A:THR:HG21 | 13       | 0.13          |
| (1,997)  | 1:79:A:TYR:H | 1:94:A:THR:HG22 | 13       | 0.13          |
| (1,997)  | 1:79:A:TYR:H | 1:94:A:THR:HG23 | 13       | 0.13          |
| (1,997)  | 1:79:A:TYR:H | 1:94:A:THR:HG21 | 36       | 0.13          |
| (1,997)  | 1:79:A:TYR:H | 1:94:A:THR:HG22 | 36       | 0.13          |
| (1,997)  | 1:79:A:TYR:H | 1:94:A:THR:HG23 | 36       | 0.13          |
| (1,997)  | 1:79:A:TYR:H | 1:94:A:THR:HG21 | 39       | 0.13          |
| (1,997)  | 1:79:A:TYR:H | 1:94:A:THR:HG22 | 39       | 0.13          |
| (1,997)  | 1:79:A:TYR:H | 1:94:A:THR:HG23 | 39       | 0.13          |
| (1,987)  | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 20       | 0.13          |
| (1,987)  | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 29       | 0.13          |
| (1,987)  | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 33       | 0.13          |
| (1,987)  | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 34       | 0.13          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 1        | 0.13          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 3        | 0.13          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 5        | 0.13          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 6        | 0.13          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 7        | 0.13          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 8        | 0.13          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 9        | 0.13          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 12       | 0.13          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 13       | 0.13          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 21       | 0.13          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 24       | 0.13          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 27       | 0.13          |
| (1,978)  | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 38       | 0.13          |
| (1,971)  | 1:21:A:VAL:H | 1:21:A:VAL:HG21 | 9        | 0.13          |
| (1,971)  | 1:21:A:VAL:H | 1:21:A:VAL:HG22 | 9        | 0.13          |
| (1,971)  | 1:21:A:VAL:H | 1:21:A:VAL:HG23 | 9        | 0.13          |
| (1,971)  | 1:21:A:VAL:H | 1:21:A:VAL:HG21 | 15       | 0.13          |
| (1,971)  | 1:21:A:VAL:H | 1:21:A:VAL:HG22 | 15       | 0.13          |
| (1,971)  | 1:21:A:VAL:H | 1:21:A:VAL:HG23 | 15       | 0.13          |
| (1,967)  | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 8        | 0.13          |
| (1,967)  | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 10       | 0.13          |
| (1,967)  | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 17       | 0.13          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,967) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 21       | 0.13          |
| (1,967) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 24       | 0.13          |
| (1,967) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 32       | 0.13          |
| (1,967) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 33       | 0.13          |
| (1,967) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 35       | 0.13          |
| (1,967) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 36       | 0.13          |
| (1,941) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 1        | 0.13          |
| (1,941) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 11       | 0.13          |
| (1,941) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 23       | 0.13          |
| (1,941) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 25       | 0.13          |
| (1,941) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 30       | 0.13          |
| (1,941) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 33       | 0.13          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 1        | 0.13          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 1        | 0.13          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 1        | 0.13          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 23       | 0.13          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 23       | 0.13          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 23       | 0.13          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 27       | 0.13          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 27       | 0.13          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 27       | 0.13          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 40       | 0.13          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 40       | 0.13          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 40       | 0.13          |
| (1,915) | 1:37:A:ASP:H | 1:37:A:ASP:HA   | 40       | 0.13          |
| (1,899) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 5        | 0.13          |
| (1,899) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 6        | 0.13          |
| (1,899) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 7        | 0.13          |
| (1,899) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 19       | 0.13          |
| (1,899) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 31       | 0.13          |
| (1,899) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 38       | 0.13          |
| (1,889) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 20       | 0.13          |
| (1,889) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 28       | 0.13          |
| (1,888) | 1:80:A:SER:H | 1:43:A:TYR:HB3  | 14       | 0.13          |
| (1,888) | 1:80:A:SER:H | 1:43:A:TYR:HB3  | 23       | 0.13          |
| (1,888) | 1:80:A:SER:H | 1:43:A:TYR:HB3  | 39       | 0.13          |
| (1,871) | 1:8:A:GLU:H  | 1:9:A:PRO:HD3   | 16       | 0.13          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 21       | 0.13          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 21       | 0.13          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 21       | 0.13          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 24       | 0.13          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 24       | 0.13          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 24       | 0.13          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 25       | 0.13          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 25       | 0.13          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 25       | 0.13          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 28       | 0.13          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 28       | 0.13          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 28       | 0.13          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 29       | 0.13          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 29       | 0.13          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 29       | 0.13          |
| (1,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB   | 12       | 0.13          |
| (1,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB   | 16       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 3        | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 3        | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 3        | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 6        | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 6        | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 6        | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 7        | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 7        | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 7        | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 8        | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 8        | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 8        | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 11       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 11       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 11       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 12       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 12       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 12       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 13       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 13       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 13       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 14       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 14       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 14       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 16       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 16       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 16       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 17       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 17       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 17       | 0.13          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 19       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 19       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 19       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 21       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 21       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 21       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 23       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 23       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 23       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 24       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 24       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 24       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 25       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 25       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 25       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 29       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 29       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 29       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 30       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 30       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 30       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 33       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 33       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 33       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 34       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 34       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 34       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 36       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 36       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 36       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 37       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 37       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 37       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 38       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 38       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 38       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG11 | 40       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG12 | 40       | 0.13          |
| (1,809) | 1:78:A:VAL:H | 1:78:A:VAL:HG13 | 40       | 0.13          |
| (1,726) | 1:49:A:LEU:H | 1:48:A:GLU:HG3  | 1        | 0.13          |
| (1,726) | 1:49:A:LEU:H | 1:48:A:GLU:HG3  | 3        | 0.13          |
| (1,726) | 1:49:A:LEU:H | 1:48:A:GLU:HG3  | 8        | 0.13          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 13       | 0.13          |
| (1,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 14       | 0.13          |
| (1,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 17       | 0.13          |
| (1,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 18       | 0.13          |
| (1,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 28       | 0.13          |
| (1,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 31       | 0.13          |
| (1,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 33       | 0.13          |
| (1,709) | 1:16:A:ILE:H  | 1:31:A:CYS:HB2  | 3        | 0.13          |
| (1,709) | 1:16:A:ILE:H  | 1:31:A:CYS:HB2  | 5        | 0.13          |
| (1,661) | 1:7:A:ALA:H   | 1:6:A:THR:HA    | 1        | 0.13          |
| (1,661) | 1:7:A:ALA:H   | 1:6:A:THR:HA    | 11       | 0.13          |
| (1,661) | 1:7:A:ALA:H   | 1:6:A:THR:HA    | 17       | 0.13          |
| (1,661) | 1:7:A:ALA:H   | 1:6:A:THR:HA    | 40       | 0.13          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 5        | 0.13          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 10       | 0.13          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 11       | 0.13          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 19       | 0.13          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 23       | 0.13          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 26       | 0.13          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 27       | 0.13          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 2        | 0.13          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 4        | 0.13          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 5        | 0.13          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 6        | 0.13          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 7        | 0.13          |
| (1,609) | 1:43:A:TYR:H  | 1:42:A:TRP:HB2  | 6        | 0.13          |
| (1,591) | 1:3:A:ASP:H   | 1:3:A:ASP:HA    | 16       | 0.13          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 10       | 0.13          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 10       | 0.13          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 10       | 0.13          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 14       | 0.13          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 14       | 0.13          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 14       | 0.13          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 18       | 0.13          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 18       | 0.13          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 18       | 0.13          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 19       | 0.13          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 19       | 0.13          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 19       | 0.13          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 20       | 0.13          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 20       | 0.13          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 20       | 0.13          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 26       | 0.13          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 26       | 0.13          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 26       | 0.13          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 35       | 0.13          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 35       | 0.13          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 35       | 0.13          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 39       | 0.13          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 39       | 0.13          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 39       | 0.13          |
| (1,560) | 1:47:A:THR:H | 1:47:A:THR:HA   | 5        | 0.13          |
| (1,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1  | 24       | 0.13          |
| (1,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2  | 24       | 0.13          |
| (1,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1  | 40       | 0.13          |
| (1,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2  | 40       | 0.13          |
| (1,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 3        | 0.13          |
| (1,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 6        | 0.13          |
| (1,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 9        | 0.13          |
| (1,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 11       | 0.13          |
| (1,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 14       | 0.13          |
| (1,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 15       | 0.13          |
| (1,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 19       | 0.13          |
| (1,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 21       | 0.13          |
| (1,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 22       | 0.13          |
| (1,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 28       | 0.13          |
| (1,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 7        | 0.13          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 6        | 0.13          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 2        | 0.13          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 10       | 0.13          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 18       | 0.13          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 20       | 0.13          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 22       | 0.13          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 38       | 0.13          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 4        | 0.13          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 10       | 0.13          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 15       | 0.13          |
| (1,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 16       | 0.13          |
| (1,419) | 1:69:A:HIS:H | 1:54:A:LYS:HA   | 6        | 0.13          |
| (1,419) | 1:69:A:HIS:H | 1:54:A:LYS:HA   | 18       | 0.13          |
| (1,410) | 1:96:A:GLU:H | 1:18:A:ASN:HD21 | 33       | 0.13          |
| (1,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD21 | 23       | 0.13          |
| (1,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD22 | 23       | 0.13          |
| (1,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD23 | 23       | 0.13          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD21 | 27       | 0.13          |
| (1,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD22 | 27       | 0.13          |
| (1,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD23 | 27       | 0.13          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 9        | 0.13          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 10       | 0.13          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 6        | 0.13          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 6        | 0.13          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 6        | 0.13          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 12       | 0.13          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 12       | 0.13          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 12       | 0.13          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 13       | 0.13          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 13       | 0.13          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 13       | 0.13          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 29       | 0.13          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 29       | 0.13          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 29       | 0.13          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 39       | 0.13          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 39       | 0.13          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 39       | 0.13          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 6        | 0.13          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 6        | 0.13          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 6        | 0.13          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 17       | 0.13          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 17       | 0.13          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 17       | 0.13          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 20       | 0.13          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 20       | 0.13          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 20       | 0.13          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 31       | 0.13          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 31       | 0.13          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 31       | 0.13          |
| (1,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 9        | 0.13          |
| (1,368) | 1:18:A:ASN:H | 1:17:A:GLN:HB3  | 28       | 0.13          |
| (1,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD1  | 3        | 0.13          |
| (1,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD2  | 3        | 0.13          |
| (1,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD1  | 4        | 0.13          |
| (1,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD2  | 4        | 0.13          |
| (1,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD1  | 36       | 0.13          |
| (1,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD2  | 36       | 0.13          |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 2        | 0.13          |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 18       | 0.13          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 19       | 0.13          |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 33       | 0.13          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 16       | 0.13          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 16       | 0.13          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 16       | 0.13          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 29       | 0.13          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 29       | 0.13          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 29       | 0.13          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 40       | 0.13          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 40       | 0.13          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 40       | 0.13          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 12       | 0.13          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 13       | 0.13          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 15       | 0.13          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 22       | 0.13          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 24       | 0.13          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 28       | 0.13          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 36       | 0.13          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1  | 7        | 0.13          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2  | 7        | 0.13          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1  | 8        | 0.13          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2  | 8        | 0.13          |
| (1,201) | 1:90:A:GLU:H | 1:89:A:GLY:HA2  | 7        | 0.13          |
| (1,201) | 1:90:A:GLU:H | 1:89:A:GLY:HA2  | 22       | 0.13          |
| (1,201) | 1:90:A:GLU:H | 1:89:A:GLY:HA2  | 23       | 0.13          |
| (1,201) | 1:90:A:GLU:H | 1:89:A:GLY:HA2  | 29       | 0.13          |
| (1,201) | 1:90:A:GLU:H | 1:89:A:GLY:HA2  | 31       | 0.13          |
| (1,201) | 1:90:A:GLU:H | 1:89:A:GLY:HA2  | 32       | 0.13          |
| (1,199) | 1:90:A:GLU:H | 1:10:A:ILE:HG21 | 6        | 0.13          |
| (1,199) | 1:90:A:GLU:H | 1:10:A:ILE:HG22 | 6        | 0.13          |
| (1,199) | 1:90:A:GLU:H | 1:10:A:ILE:HG23 | 6        | 0.13          |
| (1,199) | 1:90:A:GLU:H | 1:10:A:ILE:HG21 | 31       | 0.13          |
| (1,199) | 1:90:A:GLU:H | 1:10:A:ILE:HG22 | 31       | 0.13          |
| (1,199) | 1:90:A:GLU:H | 1:10:A:ILE:HG23 | 31       | 0.13          |
| (1,148) | 1:45:A:GLY:H | 1:46:A:PRO:HD2  | 21       | 0.13          |
| (1,148) | 1:45:A:GLY:H | 1:46:A:PRO:HD2  | 24       | 0.13          |
| (1,148) | 1:45:A:GLY:H | 1:46:A:PRO:HD2  | 31       | 0.13          |
| (1,148) | 1:45:A:GLY:H | 1:46:A:PRO:HD2  | 34       | 0.13          |
| (1,148) | 1:45:A:GLY:H | 1:46:A:PRO:HD2  | 36       | 0.13          |
| (1,111) | 1:63:A:CYS:H | 1:60:A:ASP:H    | 19       | 0.13          |
| (1,48)  | 1:57:A:PHE:H | 1:57:A:PHE:HB3  | 4        | 0.13          |
| (1,48)  | 1:57:A:PHE:H | 1:57:A:PHE:HB3  | 6        | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 7        | 0.13          |
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 17       | 0.13          |
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 19       | 0.13          |
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 28       | 0.13          |
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 34       | 0.13          |
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 35       | 0.13          |
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 36       | 0.13          |
| (1,48)   | 1:57:A:PHE:H   | 1:57:A:PHE:HB3  | 39       | 0.13          |
| (1,37)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3  | 22       | 0.13          |
| (1,37)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3  | 23       | 0.13          |
| (1,37)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3  | 24       | 0.13          |
| (1,37)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3  | 28       | 0.13          |
| (1,37)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3  | 30       | 0.13          |
| (1,37)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3  | 34       | 0.13          |
| (1,37)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3  | 35       | 0.13          |
| (1,37)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3  | 36       | 0.13          |
| (1,37)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3  | 38       | 0.13          |
| (1,35)   | 1:88:A:ARG:H   | 1:88:A:ARG:HG2  | 15       | 0.13          |
| (1,35)   | 1:88:A:ARG:H   | 1:88:A:ARG:HG2  | 19       | 0.13          |
| (1,35)   | 1:88:A:ARG:H   | 1:88:A:ARG:HG2  | 20       | 0.13          |
| (1,25)   | 1:89:A:GLY:H   | 1:88:A:ARG:HB3  | 8        | 0.13          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 9        | 0.12          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 9        | 0.12          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 24       | 0.12          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 24       | 0.12          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 25       | 0.12          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 25       | 0.12          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 27       | 0.12          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 27       | 0.12          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 29       | 0.12          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 29       | 0.12          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 34       | 0.12          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 34       | 0.12          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 36       | 0.12          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 36       | 0.12          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 38       | 0.12          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 38       | 0.12          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 4        | 0.12          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 4        | 0.12          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 4        | 0.12          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 4        | 0.12          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 4        | 0.12          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 4        | 0.12          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 22       | 0.12          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 22       | 0.12          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 22       | 0.12          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 22       | 0.12          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 22       | 0.12          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 22       | 0.12          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 26       | 0.12          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 26       | 0.12          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 26       | 0.12          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 26       | 0.12          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 26       | 0.12          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 26       | 0.12          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 31       | 0.12          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 31       | 0.12          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 31       | 0.12          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 31       | 0.12          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 31       | 0.12          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 31       | 0.12          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 36       | 0.12          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 36       | 0.12          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 36       | 0.12          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 36       | 0.12          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 36       | 0.12          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 36       | 0.12          |
| (3,3203) | 1:42:A:TRP:HZ2 | 1:30:A:GLU:HA   | 8        | 0.12          |
| (3,3203) | 1:42:A:TRP:HZ2 | 1:30:A:GLU:HA   | 20       | 0.12          |
| (3,3203) | 1:42:A:TRP:HZ2 | 1:30:A:GLU:HA   | 23       | 0.12          |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG21 | 5        | 0.12          |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG22 | 5        | 0.12          |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG23 | 5        | 0.12          |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG21 | 14       | 0.12          |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG22 | 14       | 0.12          |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG23 | 14       | 0.12          |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG21 | 27       | 0.12          |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG22 | 27       | 0.12          |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG23 | 27       | 0.12          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 11       | 0.12          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 11       | 0.12          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 11       | 0.12          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 11       | 0.12          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 17       | 0.12          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2 | 17       | 0.12          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1 | 17       | 0.12          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2 | 17       | 0.12          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1 | 20       | 0.12          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2 | 20       | 0.12          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1 | 20       | 0.12          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2 | 20       | 0.12          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1 | 23       | 0.12          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2 | 23       | 0.12          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1 | 23       | 0.12          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2 | 23       | 0.12          |
| (3,3191) | 1:43:A:TYR:HD1 | 1:44:A:LYS:H   | 3        | 0.12          |
| (3,3191) | 1:43:A:TYR:HD2 | 1:44:A:LYS:H   | 3        | 0.12          |
| (3,3191) | 1:43:A:TYR:HD1 | 1:44:A:LYS:H   | 4        | 0.12          |
| (3,3191) | 1:43:A:TYR:HD2 | 1:44:A:LYS:H   | 4        | 0.12          |
| (3,3191) | 1:43:A:TYR:HD1 | 1:44:A:LYS:H   | 5        | 0.12          |
| (3,3191) | 1:43:A:TYR:HD2 | 1:44:A:LYS:H   | 5        | 0.12          |
| (3,3191) | 1:43:A:TYR:HD1 | 1:44:A:LYS:H   | 12       | 0.12          |
| (3,3191) | 1:43:A:TYR:HD2 | 1:44:A:LYS:H   | 12       | 0.12          |
| (3,3191) | 1:43:A:TYR:HD1 | 1:44:A:LYS:H   | 15       | 0.12          |
| (3,3191) | 1:43:A:TYR:HD2 | 1:44:A:LYS:H   | 15       | 0.12          |
| (3,3191) | 1:43:A:TYR:HD1 | 1:44:A:LYS:H   | 20       | 0.12          |
| (3,3191) | 1:43:A:TYR:HD2 | 1:44:A:LYS:H   | 20       | 0.12          |
| (3,3191) | 1:43:A:TYR:HD1 | 1:44:A:LYS:H   | 27       | 0.12          |
| (3,3191) | 1:43:A:TYR:HD2 | 1:44:A:LYS:H   | 27       | 0.12          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1 | 7        | 0.12          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2 | 7        | 0.12          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3 | 7        | 0.12          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1 | 10       | 0.12          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2 | 10       | 0.12          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3 | 10       | 0.12          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1 | 34       | 0.12          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2 | 34       | 0.12          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3 | 34       | 0.12          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1 | 38       | 0.12          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2 | 38       | 0.12          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3 | 38       | 0.12          |
| (3,3164) | 1:42:A:TRP:HD1 | 1:41:A:THR:HA  | 29       | 0.12          |
| (3,3164) | 1:42:A:TRP:HD1 | 1:41:A:THR:HA  | 40       | 0.12          |
| (3,3143) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3 | 9        | 0.12          |
| (3,3143) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3 | 9        | 0.12          |
| (3,3143) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3 | 22       | 0.12          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3143) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 22       | 0.12          |
| (3,3143) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3  | 24       | 0.12          |
| (3,3143) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 24       | 0.12          |
| (3,3143) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3  | 32       | 0.12          |
| (3,3143) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 32       | 0.12          |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2  | 17       | 0.12          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2  | 17       | 0.12          |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2  | 20       | 0.12          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2  | 20       | 0.12          |
| (3,3139) | 1:65:A:TYR:HE1 | 1:60:A:ASP:HB3  | 21       | 0.12          |
| (3,3139) | 1:65:A:TYR:HE2 | 1:60:A:ASP:HB3  | 21       | 0.12          |
| (3,3139) | 1:65:A:TYR:HE1 | 1:60:A:ASP:HB3  | 23       | 0.12          |
| (3,3139) | 1:65:A:TYR:HE2 | 1:60:A:ASP:HB3  | 23       | 0.12          |
| (3,3138) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB2  | 2        | 0.12          |
| (3,3138) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB2  | 2        | 0.12          |
| (3,3138) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB2  | 12       | 0.12          |
| (3,3138) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB2  | 12       | 0.12          |
| (3,3138) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB2  | 13       | 0.12          |
| (3,3138) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB2  | 13       | 0.12          |
| (3,3138) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB2  | 21       | 0.12          |
| (3,3138) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB2  | 21       | 0.12          |
| (3,3137) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3  | 13       | 0.12          |
| (3,3137) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3  | 13       | 0.12          |
| (3,3137) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3  | 28       | 0.12          |
| (3,3137) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3  | 28       | 0.12          |
| (3,3137) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3  | 37       | 0.12          |
| (3,3137) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3  | 37       | 0.12          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 8        | 0.12          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 8        | 0.12          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 8        | 0.12          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 8        | 0.12          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 8        | 0.12          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 8        | 0.12          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 29       | 0.12          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 29       | 0.12          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 29       | 0.12          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 29       | 0.12          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 29       | 0.12          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 29       | 0.12          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 33       | 0.12          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 33       | 0.12          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 33       | 0.12          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 33       | 0.12          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 33       | 0.12          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 33       | 0.12          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 14       | 0.12          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 14       | 0.12          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 14       | 0.12          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 14       | 0.12          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 14       | 0.12          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 14       | 0.12          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 28       | 0.12          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 28       | 0.12          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 28       | 0.12          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 28       | 0.12          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 28       | 0.12          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 28       | 0.12          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 29       | 0.12          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 29       | 0.12          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 29       | 0.12          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 29       | 0.12          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 29       | 0.12          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 29       | 0.12          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 39       | 0.12          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 39       | 0.12          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 39       | 0.12          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 39       | 0.12          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 39       | 0.12          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 39       | 0.12          |
| (3,3110) | 1:79:A:TYR:HE1 | 1:66:A:MET:HE1  | 1        | 0.12          |
| (3,3110) | 1:79:A:TYR:HE1 | 1:66:A:MET:HE2  | 1        | 0.12          |
| (3,3110) | 1:79:A:TYR:HE1 | 1:66:A:MET:HE3  | 1        | 0.12          |
| (3,3110) | 1:79:A:TYR:HE2 | 1:66:A:MET:HE1  | 1        | 0.12          |
| (3,3110) | 1:79:A:TYR:HE2 | 1:66:A:MET:HE2  | 1        | 0.12          |
| (3,3110) | 1:79:A:TYR:HE2 | 1:66:A:MET:HE3  | 1        | 0.12          |
| (3,3110) | 1:79:A:TYR:HE1 | 1:66:A:MET:HE1  | 5        | 0.12          |
| (3,3110) | 1:79:A:TYR:HE1 | 1:66:A:MET:HE2  | 5        | 0.12          |
| (3,3110) | 1:79:A:TYR:HE1 | 1:66:A:MET:HE3  | 5        | 0.12          |
| (3,3110) | 1:79:A:TYR:HE2 | 1:66:A:MET:HE1  | 5        | 0.12          |
| (3,3110) | 1:79:A:TYR:HE2 | 1:66:A:MET:HE2  | 5        | 0.12          |
| (3,3110) | 1:79:A:TYR:HE2 | 1:66:A:MET:HE3  | 5        | 0.12          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 13       | 0.12          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 13       | 0.12          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 13       | 0.12          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2 | 13       | 0.12          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1 | 18       | 0.12          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2 | 18       | 0.12          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1 | 18       | 0.12          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2 | 18       | 0.12          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1 | 26       | 0.12          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2 | 26       | 0.12          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1 | 26       | 0.12          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2 | 26       | 0.12          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1 | 29       | 0.12          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2 | 29       | 0.12          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1 | 29       | 0.12          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2 | 29       | 0.12          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1 | 39       | 0.12          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2 | 39       | 0.12          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1 | 39       | 0.12          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2 | 39       | 0.12          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1 | 3        | 0.12          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2 | 3        | 0.12          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1 | 3        | 0.12          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2 | 3        | 0.12          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1 | 3        | 0.12          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2 | 3        | 0.12          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1 | 5        | 0.12          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2 | 5        | 0.12          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1 | 5        | 0.12          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2 | 5        | 0.12          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1 | 5        | 0.12          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2 | 5        | 0.12          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1 | 15       | 0.12          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2 | 15       | 0.12          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1 | 15       | 0.12          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2 | 15       | 0.12          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1 | 15       | 0.12          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2 | 15       | 0.12          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1 | 23       | 0.12          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2 | 23       | 0.12          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1 | 23       | 0.12          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2 | 23       | 0.12          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1 | 23       | 0.12          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2 | 23       | 0.12          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1 | 26       | 0.12          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 26       | 0.12          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 26       | 0.12          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 26       | 0.12          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 26       | 0.12          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 26       | 0.12          |
| (3,3092) | 1:7:A:ALA:HB1  | 1:88:A:ARG:HD3  | 4        | 0.12          |
| (3,3092) | 1:7:A:ALA:HB2  | 1:88:A:ARG:HD3  | 4        | 0.12          |
| (3,3092) | 1:7:A:ALA:HB3  | 1:88:A:ARG:HD3  | 4        | 0.12          |
| (3,3092) | 1:7:A:ALA:HB1  | 1:88:A:ARG:HD3  | 5        | 0.12          |
| (3,3092) | 1:7:A:ALA:HB2  | 1:88:A:ARG:HD3  | 5        | 0.12          |
| (3,3092) | 1:7:A:ALA:HB3  | 1:88:A:ARG:HD3  | 5        | 0.12          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 14       | 0.12          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 14       | 0.12          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 14       | 0.12          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 20       | 0.12          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 20       | 0.12          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 20       | 0.12          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 23       | 0.12          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 23       | 0.12          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 23       | 0.12          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 25       | 0.12          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 25       | 0.12          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 25       | 0.12          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 30       | 0.12          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 30       | 0.12          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 30       | 0.12          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 35       | 0.12          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 35       | 0.12          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 35       | 0.12          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 36       | 0.12          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 36       | 0.12          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 36       | 0.12          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 39       | 0.12          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 39       | 0.12          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 39       | 0.12          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 9        | 0.12          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 9        | 0.12          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 30       | 0.12          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 30       | 0.12          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 33       | 0.12          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 33       | 0.12          |
| (3,3048) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG21 | 24       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,3048) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG22 | 24       | 0.12          |
| (3,3048) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG23 | 24       | 0.12          |
| (3,3048) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG21 | 28       | 0.12          |
| (3,3048) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG22 | 28       | 0.12          |
| (3,3048) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG23 | 28       | 0.12          |
| (3,3048) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG21 | 39       | 0.12          |
| (3,3048) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG22 | 39       | 0.12          |
| (3,3048) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG23 | 39       | 0.12          |
| (3,3041) | 1:44:A:LYS:HE2  | 1:79:A:TYR:HE1  | 33       | 0.12          |
| (3,3041) | 1:44:A:LYS:HE2  | 1:79:A:TYR:HE2  | 33       | 0.12          |
| (3,3021) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 4        | 0.12          |
| (3,3021) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 4        | 0.12          |
| (3,3021) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 6        | 0.12          |
| (3,3021) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 6        | 0.12          |
| (3,3021) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 15       | 0.12          |
| (3,3021) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 15       | 0.12          |
| (3,3021) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 16       | 0.12          |
| (3,3021) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 16       | 0.12          |
| (3,3021) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 31       | 0.12          |
| (3,3021) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 31       | 0.12          |
| (3,3021) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 39       | 0.12          |
| (3,3021) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 39       | 0.12          |
| (3,3020) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG21 | 11       | 0.12          |
| (3,3020) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG22 | 11       | 0.12          |
| (3,3020) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG23 | 11       | 0.12          |
| (3,3020) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG21 | 12       | 0.12          |
| (3,3020) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG22 | 12       | 0.12          |
| (3,3020) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG23 | 12       | 0.12          |
| (3,3020) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG21 | 35       | 0.12          |
| (3,3020) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG22 | 35       | 0.12          |
| (3,3020) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG23 | 35       | 0.12          |
| (3,3020) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG21 | 38       | 0.12          |
| (3,3020) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG22 | 38       | 0.12          |
| (3,3020) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG23 | 38       | 0.12          |
| (3,3019) | 1:30:A:GLU:HB2  | 1:14:A:LYS:HE2  | 2        | 0.12          |
| (3,3019) | 1:30:A:GLU:HB2  | 1:14:A:LYS:HE2  | 3        | 0.12          |
| (3,3019) | 1:30:A:GLU:HB2  | 1:14:A:LYS:HE2  | 19       | 0.12          |
| (3,3019) | 1:30:A:GLU:HB2  | 1:14:A:LYS:HE2  | 40       | 0.12          |
| (3,3017) | 1:102:A:ARG:HD3 | 1:102:A:ARG:HB2 | 25       | 0.12          |
| (3,3004) | 1:15:A:ARG:HG2  | 1:93:A:SER:HB3  | 21       | 0.12          |
| (3,3004) | 1:15:A:ARG:HG2  | 1:93:A:SER:HB3  | 22       | 0.12          |
| (3,3004) | 1:15:A:ARG:HG2  | 1:93:A:SER:HB3  | 33       | 0.12          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,2982) | 1:65:A:TYR:HA  | 1:42:A:TRP:HZ2 | 4        | 0.12          |
| (3,2982) | 1:65:A:TYR:HA  | 1:42:A:TRP:HZ2 | 10       | 0.12          |
| (3,2982) | 1:65:A:TYR:HA  | 1:42:A:TRP:HZ2 | 26       | 0.12          |
| (3,2982) | 1:65:A:TYR:HA  | 1:42:A:TRP:HZ2 | 39       | 0.12          |
| (3,2982) | 1:65:A:TYR:HA  | 1:42:A:TRP:HZ2 | 40       | 0.12          |
| (3,2975) | 1:44:A:LYS:HE3 | 1:44:A:LYS:HD2 | 35       | 0.12          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 1        | 0.12          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 9        | 0.12          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 11       | 0.12          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 16       | 0.12          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 17       | 0.12          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 22       | 0.12          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 25       | 0.12          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 31       | 0.12          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 37       | 0.12          |
| (3,2961) | 1:98:A:LYS:HB3 | 1:98:A:LYS:HG2 | 38       | 0.12          |
| (3,2957) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 2        | 0.12          |
| (3,2957) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 11       | 0.12          |
| (3,2957) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 18       | 0.12          |
| (3,2957) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 19       | 0.12          |
| (3,2957) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 20       | 0.12          |
| (3,2957) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 22       | 0.12          |
| (3,2957) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 24       | 0.12          |
| (3,2957) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 32       | 0.12          |
| (3,2957) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 35       | 0.12          |
| (3,2957) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA   | 38       | 0.12          |
| (3,2949) | 1:90:A:GLU:HA  | 1:84:A:ARG:HA  | 15       | 0.12          |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1 | 9        | 0.12          |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2 | 9        | 0.12          |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1 | 22       | 0.12          |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2 | 22       | 0.12          |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1 | 24       | 0.12          |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2 | 24       | 0.12          |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1 | 32       | 0.12          |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2 | 32       | 0.12          |
| (3,2938) | 1:26:A:SER:HA  | 1:70:A:ASN:H   | 9        | 0.12          |
| (3,2938) | 1:26:A:SER:HA  | 1:70:A:ASN:H   | 13       | 0.12          |
| (3,2938) | 1:26:A:SER:HA  | 1:70:A:ASN:H   | 19       | 0.12          |
| (3,2938) | 1:26:A:SER:HA  | 1:70:A:ASN:H   | 20       | 0.12          |
| (3,2938) | 1:26:A:SER:HA  | 1:70:A:ASN:H   | 27       | 0.12          |
| (3,2938) | 1:26:A:SER:HA  | 1:70:A:ASN:H   | 33       | 0.12          |
| (3,2910) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HD2 | 16       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 4        | 0.12          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 5        | 0.12          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 6        | 0.12          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 11       | 0.12          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 12       | 0.12          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 13       | 0.12          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 16       | 0.12          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 17       | 0.12          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 21       | 0.12          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 24       | 0.12          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 27       | 0.12          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 29       | 0.12          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 33       | 0.12          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 35       | 0.12          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 38       | 0.12          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 39       | 0.12          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 40       | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 1        | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 2        | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 3        | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 4        | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 6        | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 8        | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 10       | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 11       | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 12       | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 13       | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 14       | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 15       | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 16       | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 17       | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 18       | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 21       | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 22       | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 23       | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 24       | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 25       | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 26       | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 27       | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 28       | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 30       | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 31       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 32       | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 33       | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 34       | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 35       | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 36       | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 37       | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 38       | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 39       | 0.12          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 40       | 0.12          |
| (3,2866) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 27       | 0.12          |
| (3,2848) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA   | 26       | 0.12          |
| (3,2848) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA   | 34       | 0.12          |
| (3,2829) | 1:58:A:ARG:HD3  | 1:58:A:ARG:HG2  | 21       | 0.12          |
| (3,2809) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HB2  | 6        | 0.12          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 12       | 0.12          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 13       | 0.12          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 18       | 0.12          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 20       | 0.12          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 30       | 0.12          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 35       | 0.12          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 36       | 0.12          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 37       | 0.12          |
| (3,2761) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 2        | 0.12          |
| (3,2761) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 15       | 0.12          |
| (3,2761) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 16       | 0.12          |
| (3,2761) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 17       | 0.12          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H    | 5        | 0.12          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H    | 14       | 0.12          |
| (3,2727) | 1:76:A:GLU:HB2  | 1:77:A:GLY:H    | 17       | 0.12          |
| (3,2717) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 1        | 0.12          |
| (3,2717) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 2        | 0.12          |
| (3,2717) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 3        | 0.12          |
| (3,2717) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 4        | 0.12          |
| (3,2717) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 5        | 0.12          |
| (3,2717) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 6        | 0.12          |
| (3,2717) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 10       | 0.12          |
| (3,2717) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 12       | 0.12          |
| (3,2717) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 13       | 0.12          |
| (3,2717) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 15       | 0.12          |
| (3,2717) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 16       | 0.12          |
| (3,2717) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 17       | 0.12          |
| (3,2717) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 18       | 0.12          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,2717) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 19       | 0.12          |
| (3,2717) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 21       | 0.12          |
| (3,2717) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 22       | 0.12          |
| (3,2717) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 23       | 0.12          |
| (3,2717) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 24       | 0.12          |
| (3,2717) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 25       | 0.12          |
| (3,2717) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 26       | 0.12          |
| (3,2717) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 27       | 0.12          |
| (3,2717) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 28       | 0.12          |
| (3,2717) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 30       | 0.12          |
| (3,2717) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 31       | 0.12          |
| (3,2717) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 32       | 0.12          |
| (3,2717) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 33       | 0.12          |
| (3,2717) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 34       | 0.12          |
| (3,2717) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 36       | 0.12          |
| (3,2717) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 37       | 0.12          |
| (3,2717) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 38       | 0.12          |
| (3,2717) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 40       | 0.12          |
| (3,2703) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA  | 1        | 0.12          |
| (3,2703) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA  | 10       | 0.12          |
| (3,2703) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA  | 11       | 0.12          |
| (3,2703) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA  | 15       | 0.12          |
| (3,2703) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA  | 16       | 0.12          |
| (3,2703) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA  | 21       | 0.12          |
| (3,2703) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA  | 22       | 0.12          |
| (3,2703) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA  | 25       | 0.12          |
| (3,2703) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA  | 26       | 0.12          |
| (3,2703) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA  | 27       | 0.12          |
| (3,2703) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA  | 30       | 0.12          |
| (3,2703) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA  | 32       | 0.12          |
| (3,2703) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA  | 35       | 0.12          |
| (3,2703) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA  | 40       | 0.12          |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2  | 3        | 0.12          |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2  | 12       | 0.12          |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2  | 15       | 0.12          |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2  | 25       | 0.12          |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2  | 29       | 0.12          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 1        | 0.12          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 2        | 0.12          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 3        | 0.12          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 6        | 0.12          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 7        | 0.12          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 11       | 0.12          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 12       | 0.12          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 13       | 0.12          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 14       | 0.12          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 17       | 0.12          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 18       | 0.12          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 19       | 0.12          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 20       | 0.12          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 22       | 0.12          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 25       | 0.12          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 26       | 0.12          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 27       | 0.12          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 28       | 0.12          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 29       | 0.12          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 30       | 0.12          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 31       | 0.12          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 32       | 0.12          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 33       | 0.12          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 34       | 0.12          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 36       | 0.12          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 37       | 0.12          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 38       | 0.12          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 39       | 0.12          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 40       | 0.12          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 3        | 0.12          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 3        | 0.12          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 3        | 0.12          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 8        | 0.12          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 8        | 0.12          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 8        | 0.12          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 28       | 0.12          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 28       | 0.12          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 28       | 0.12          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 39       | 0.12          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 39       | 0.12          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 39       | 0.12          |
| (3,2653) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 6        | 0.12          |
| (3,2653) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 7        | 0.12          |
| (3,2653) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 10       | 0.12          |
| (3,2653) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 15       | 0.12          |
| (3,2653) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 17       | 0.12          |
| (3,2653) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 22       | 0.12          |

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| Key      | Atom-1         | Atom-2        | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (3,2653) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H  | 23       | 0.12          |
| (3,2650) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3 | 21       | 0.12          |
| (3,2650) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3 | 22       | 0.12          |
| (3,2650) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3 | 24       | 0.12          |
| (3,2650) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3 | 32       | 0.12          |
| (3,2650) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3 | 35       | 0.12          |
| (3,2613) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H  | 6        | 0.12          |
| (3,2613) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H  | 13       | 0.12          |
| (3,2612) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H  | 6        | 0.12          |
| (3,2612) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H  | 13       | 0.12          |
| (3,2554) | 1:92:A:ARG:HA  | 1:83:A:ALA:H  | 2        | 0.12          |
| (3,2554) | 1:92:A:ARG:HA  | 1:83:A:ALA:H  | 10       | 0.12          |
| (3,2554) | 1:92:A:ARG:HA  | 1:83:A:ALA:H  | 11       | 0.12          |
| (3,2554) | 1:92:A:ARG:HA  | 1:83:A:ALA:H  | 13       | 0.12          |
| (3,2554) | 1:92:A:ARG:HA  | 1:83:A:ALA:H  | 22       | 0.12          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA | 11       | 0.12          |
| (3,2543) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA | 18       | 0.12          |
| (3,2541) | 1:73:A:PRO:HG3 | 1:73:A:PRO:HA | 22       | 0.12          |
| (3,2541) | 1:73:A:PRO:HG3 | 1:73:A:PRO:HA | 33       | 0.12          |
| (3,2541) | 1:73:A:PRO:HG3 | 1:73:A:PRO:HA | 39       | 0.12          |
| (3,2529) | 1:87:A:PRO:HB3 | 1:86:A:GLU:HA | 29       | 0.12          |
| (3,2529) | 1:87:A:PRO:HB3 | 1:86:A:GLU:HA | 35       | 0.12          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 26       | 0.12          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 28       | 0.12          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 33       | 0.12          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 21       | 0.12          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 22       | 0.12          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 23       | 0.12          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 24       | 0.12          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 25       | 0.12          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 27       | 0.12          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 30       | 0.12          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 32       | 0.12          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 34       | 0.12          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 38       | 0.12          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 40       | 0.12          |
| (3,2482) | 1:9:A:PRO:HD2  | 1:8:A:GLU:HA  | 1        | 0.12          |
| (3,2482) | 1:9:A:PRO:HD2  | 1:8:A:GLU:HA  | 20       | 0.12          |
| (3,2482) | 1:9:A:PRO:HD2  | 1:8:A:GLU:HA  | 33       | 0.12          |
| (3,2463) | 1:4:A:PRO:HD3  | 1:3:A:ASP:HA  | 8        | 0.12          |
| (3,2463) | 1:4:A:PRO:HD3  | 1:3:A:ASP:HA  | 9        | 0.12          |
| (3,2463) | 1:4:A:PRO:HD3  | 1:3:A:ASP:HA  | 25       | 0.12          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,2434) | 1:82:A:ILE:HB  | 1:41:A:THR:H    | 10       | 0.12          |
| (3,2434) | 1:82:A:ILE:HB  | 1:41:A:THR:H    | 15       | 0.12          |
| (3,2427) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD11 | 38       | 0.12          |
| (3,2427) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD12 | 38       | 0.12          |
| (3,2427) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD13 | 38       | 0.12          |
| (3,2419) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 5        | 0.12          |
| (3,2419) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 9        | 0.12          |
| (3,2419) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 11       | 0.12          |
| (3,2419) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 17       | 0.12          |
| (3,2419) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 27       | 0.12          |
| (3,2412) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2  | 15       | 0.12          |
| (3,2412) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2  | 19       | 0.12          |
| (3,2406) | 1:66:A:MET:HE1 | 1:42:A:TRP:H    | 6        | 0.12          |
| (3,2406) | 1:66:A:MET:HE2 | 1:42:A:TRP:H    | 6        | 0.12          |
| (3,2406) | 1:66:A:MET:HE3 | 1:42:A:TRP:H    | 6        | 0.12          |
| (3,2406) | 1:66:A:MET:HE1 | 1:42:A:TRP:H    | 40       | 0.12          |
| (3,2406) | 1:66:A:MET:HE2 | 1:42:A:TRP:H    | 40       | 0.12          |
| (3,2406) | 1:66:A:MET:HE3 | 1:42:A:TRP:H    | 40       | 0.12          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ   | 4        | 0.12          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ   | 4        | 0.12          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ   | 4        | 0.12          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ   | 24       | 0.12          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ   | 24       | 0.12          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ   | 24       | 0.12          |
| (3,2342) | 1:26:A:SER:HB3 | 1:27:A:ALA:H    | 11       | 0.12          |
| (3,2342) | 1:26:A:SER:HB3 | 1:27:A:ALA:H    | 30       | 0.12          |
| (3,2334) | 1:26:A:SER:HA  | 1:68:A:ILE:HG21 | 4        | 0.12          |
| (3,2334) | 1:26:A:SER:HA  | 1:68:A:ILE:HG22 | 4        | 0.12          |
| (3,2334) | 1:26:A:SER:HA  | 1:68:A:ILE:HG23 | 4        | 0.12          |
| (3,2334) | 1:26:A:SER:HA  | 1:68:A:ILE:HG21 | 22       | 0.12          |
| (3,2334) | 1:26:A:SER:HA  | 1:68:A:ILE:HG22 | 22       | 0.12          |
| (3,2334) | 1:26:A:SER:HA  | 1:68:A:ILE:HG23 | 22       | 0.12          |
| (3,2334) | 1:26:A:SER:HA  | 1:68:A:ILE:HG21 | 25       | 0.12          |
| (3,2334) | 1:26:A:SER:HA  | 1:68:A:ILE:HG22 | 25       | 0.12          |
| (3,2334) | 1:26:A:SER:HA  | 1:68:A:ILE:HG23 | 25       | 0.12          |
| (3,2290) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H    | 4        | 0.12          |
| (3,2290) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H    | 8        | 0.12          |
| (3,2290) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H    | 29       | 0.12          |
| (3,2268) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG21 | 3        | 0.12          |
| (3,2268) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG22 | 3        | 0.12          |
| (3,2268) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG23 | 3        | 0.12          |
| (3,2268) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG21 | 9        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG22 | 9        | 0.12          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG23 | 9        | 0.12          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG21 | 10       | 0.12          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG22 | 10       | 0.12          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG23 | 10       | 0.12          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG21 | 12       | 0.12          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG22 | 12       | 0.12          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG23 | 12       | 0.12          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG21 | 16       | 0.12          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG22 | 16       | 0.12          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG23 | 16       | 0.12          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG21 | 27       | 0.12          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG22 | 27       | 0.12          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG23 | 27       | 0.12          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG21 | 35       | 0.12          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG22 | 35       | 0.12          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG23 | 35       | 0.12          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG21 | 36       | 0.12          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG22 | 36       | 0.12          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG23 | 36       | 0.12          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG21 | 37       | 0.12          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG22 | 37       | 0.12          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG23 | 37       | 0.12          |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD11 | 28       | 0.12          |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD12 | 28       | 0.12          |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD13 | 28       | 0.12          |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD11 | 38       | 0.12          |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD12 | 38       | 0.12          |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD13 | 38       | 0.12          |
| (3,2153) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 16       | 0.12          |
| (3,2153) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 33       | 0.12          |
| (3,2148) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 6        | 0.12          |
| (3,2148) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 10       | 0.12          |
| (3,2148) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 22       | 0.12          |
| (3,2148) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 29       | 0.12          |
| (3,2148) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 31       | 0.12          |
| (3,2148) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 32       | 0.12          |
| (3,2148) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 36       | 0.12          |
| (3,2102) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HA   | 7        | 0.12          |
| (3,2102) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HA   | 7        | 0.12          |
| (3,2102) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HA   | 7        | 0.12          |
| (3,2102) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HA   | 30       | 0.12          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2102) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HA  | 30       | 0.12          |
| (3,2102) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HA  | 30       | 0.12          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2 | 6        | 0.12          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2 | 6        | 0.12          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2 | 6        | 0.12          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2 | 15       | 0.12          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2 | 15       | 0.12          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2 | 15       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1 | 5        | 0.12          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2 | 5        | 0.12          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1 | 5        | 0.12          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2 | 5        | 0.12          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1 | 5        | 0.12          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2 | 5        | 0.12          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1 | 8        | 0.12          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2 | 8        | 0.12          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1 | 8        | 0.12          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2 | 8        | 0.12          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1 | 8        | 0.12          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2 | 8        | 0.12          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1 | 14       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2 | 14       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1 | 14       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2 | 14       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1 | 14       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2 | 14       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1 | 21       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2 | 21       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1 | 21       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2 | 21       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1 | 21       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2 | 21       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1 | 22       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2 | 22       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1 | 22       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2 | 22       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1 | 22       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2 | 22       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1 | 25       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2 | 25       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1 | 25       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2 | 25       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1  | 25       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2  | 25       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1  | 31       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2  | 31       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1  | 31       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2  | 31       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1  | 31       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2  | 31       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1  | 36       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2  | 36       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1  | 36       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2  | 36       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1  | 36       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2  | 36       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1  | 37       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2  | 37       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1  | 37       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2  | 37       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1  | 37       | 0.12          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2  | 37       | 0.12          |
| (3,2081) | 1:97:A:LEU:HD11 | 1:21:A:VAL:HB   | 9        | 0.12          |
| (3,2081) | 1:97:A:LEU:HD12 | 1:21:A:VAL:HB   | 9        | 0.12          |
| (3,2081) | 1:97:A:LEU:HD13 | 1:21:A:VAL:HB   | 9        | 0.12          |
| (3,2073) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 16       | 0.12          |
| (3,2073) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 16       | 0.12          |
| (3,2073) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 16       | 0.12          |
| (3,2073) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 40       | 0.12          |
| (3,2073) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 40       | 0.12          |
| (3,2073) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 40       | 0.12          |
| (3,2059) | 1:78:A:VAL:HG11 | 1:96:A:GLU:HG2  | 38       | 0.12          |
| (3,2059) | 1:78:A:VAL:HG12 | 1:96:A:GLU:HG2  | 38       | 0.12          |
| (3,2059) | 1:78:A:VAL:HG13 | 1:96:A:GLU:HG2  | 38       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD21 | 19       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD22 | 19       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD23 | 19       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD21 | 19       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD22 | 19       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD23 | 19       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD21 | 19       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD22 | 19       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD23 | 19       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD21 | 25       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD22 | 25       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD23 | 25       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD21 | 25       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD22 | 25       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD23 | 25       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD21 | 25       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD22 | 25       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD23 | 25       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD21 | 30       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD22 | 30       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD23 | 30       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD21 | 30       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD22 | 30       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD23 | 30       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD21 | 30       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD22 | 30       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD23 | 30       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD21 | 32       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD22 | 32       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD23 | 32       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD21 | 32       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD22 | 32       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD23 | 32       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD21 | 32       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD22 | 32       | 0.12          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD23 | 32       | 0.12          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1  | 6        | 0.12          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2  | 6        | 0.12          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1  | 6        | 0.12          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2  | 6        | 0.12          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1  | 6        | 0.12          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2  | 6        | 0.12          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1  | 12       | 0.12          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2  | 12       | 0.12          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1  | 12       | 0.12          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2  | 12       | 0.12          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1  | 12       | 0.12          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2  | 12       | 0.12          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1  | 24       | 0.12          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2  | 24       | 0.12          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1  | 24       | 0.12          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2  | 24       | 0.12          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 24       | 0.12          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 24       | 0.12          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 40       | 0.12          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 40       | 0.12          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 40       | 0.12          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 40       | 0.12          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 40       | 0.12          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 40       | 0.12          |
| (3,2027) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ  | 34       | 0.12          |
| (3,2027) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ  | 34       | 0.12          |
| (3,2027) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ  | 34       | 0.12          |
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 3        | 0.12          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 3        | 0.12          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 3        | 0.12          |
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 5        | 0.12          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 5        | 0.12          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 5        | 0.12          |
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 7        | 0.12          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 7        | 0.12          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 7        | 0.12          |
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 20       | 0.12          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 20       | 0.12          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 20       | 0.12          |
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 21       | 0.12          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 21       | 0.12          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 21       | 0.12          |
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 23       | 0.12          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 23       | 0.12          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 23       | 0.12          |
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 25       | 0.12          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 25       | 0.12          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 25       | 0.12          |
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 32       | 0.12          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 32       | 0.12          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 32       | 0.12          |
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 34       | 0.12          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 34       | 0.12          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 34       | 0.12          |
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 36       | 0.12          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 36       | 0.12          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 36       | 0.12          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 9        | 0.12          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 9        | 0.12          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 9        | 0.12          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 9        | 0.12          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 9        | 0.12          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 9        | 0.12          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 27       | 0.12          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 27       | 0.12          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 27       | 0.12          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 27       | 0.12          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 27       | 0.12          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 27       | 0.12          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 31       | 0.12          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 31       | 0.12          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 31       | 0.12          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 31       | 0.12          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 31       | 0.12          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 31       | 0.12          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 37       | 0.12          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 37       | 0.12          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 37       | 0.12          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 37       | 0.12          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 37       | 0.12          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 37       | 0.12          |
| (3,2019) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD1 | 15       | 0.12          |
| (3,2019) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD2 | 15       | 0.12          |
| (3,2019) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD1 | 33       | 0.12          |
| (3,2019) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD2 | 33       | 0.12          |
| (3,2016) | 1:40:A:VAL:HG11 | 1:64:A:HIS:HD2 | 27       | 0.12          |
| (3,2016) | 1:40:A:VAL:HG12 | 1:64:A:HIS:HD2 | 27       | 0.12          |
| (3,2016) | 1:40:A:VAL:HG13 | 1:64:A:HIS:HD2 | 27       | 0.12          |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1 | 6        | 0.12          |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2 | 6        | 0.12          |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3 | 6        | 0.12          |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1 | 6        | 0.12          |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2 | 6        | 0.12          |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3 | 6        | 0.12          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1 | 6        | 0.12          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2 | 6        | 0.12          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3 | 6        | 0.12          |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1 | 23       | 0.12          |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2 | 23       | 0.12          |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3 | 23       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1  | 23       | 0.12          |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2  | 23       | 0.12          |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3  | 23       | 0.12          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1  | 23       | 0.12          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2  | 23       | 0.12          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3  | 23       | 0.12          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 3        | 0.12          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 4        | 0.12          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 21       | 0.12          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 24       | 0.12          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 39       | 0.12          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 40       | 0.12          |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 12       | 0.12          |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 12       | 0.12          |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 12       | 0.12          |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 13       | 0.12          |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 13       | 0.12          |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 13       | 0.12          |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 40       | 0.12          |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 40       | 0.12          |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 40       | 0.12          |
| (3,1997) | 1:21:A:VAL:HG11 | 1:25:A:GLN:HG3  | 37       | 0.12          |
| (3,1997) | 1:21:A:VAL:HG12 | 1:25:A:GLN:HG3  | 37       | 0.12          |
| (3,1997) | 1:21:A:VAL:HG13 | 1:25:A:GLN:HG3  | 37       | 0.12          |
| (3,1993) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 1        | 0.12          |
| (3,1993) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 1        | 0.12          |
| (3,1993) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 1        | 0.12          |
| (3,1993) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 16       | 0.12          |
| (3,1993) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 16       | 0.12          |
| (3,1993) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 16       | 0.12          |
| (3,1993) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 19       | 0.12          |
| (3,1993) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 19       | 0.12          |
| (3,1993) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 19       | 0.12          |
| (3,1993) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 35       | 0.12          |
| (3,1993) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 35       | 0.12          |
| (3,1993) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 35       | 0.12          |
| (3,1993) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 38       | 0.12          |
| (3,1993) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 38       | 0.12          |
| (3,1993) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 38       | 0.12          |
| (3,1969) | 1:36:A:ASP:HB3  | 1:62:A:ARG:HA   | 31       | 0.12          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 20       | 0.12          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 36       | 0.12          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1955) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB1 | 15       | 0.12          |
| (3,1955) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB2 | 15       | 0.12          |
| (3,1955) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB3 | 15       | 0.12          |
| (3,1955) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB1 | 15       | 0.12          |
| (3,1955) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB2 | 15       | 0.12          |
| (3,1955) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB3 | 15       | 0.12          |
| (3,1955) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB1 | 15       | 0.12          |
| (3,1955) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB2 | 15       | 0.12          |
| (3,1955) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB3 | 15       | 0.12          |
| (3,1955) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB1 | 34       | 0.12          |
| (3,1955) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB2 | 34       | 0.12          |
| (3,1955) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB3 | 34       | 0.12          |
| (3,1955) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB1 | 34       | 0.12          |
| (3,1955) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB2 | 34       | 0.12          |
| (3,1955) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB3 | 34       | 0.12          |
| (3,1955) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB1 | 34       | 0.12          |
| (3,1955) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB2 | 34       | 0.12          |
| (3,1955) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB3 | 34       | 0.12          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 8        | 0.12          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 8        | 0.12          |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 8        | 0.12          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 11       | 0.12          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 11       | 0.12          |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 11       | 0.12          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 12       | 0.12          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 12       | 0.12          |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 12       | 0.12          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 24       | 0.12          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 24       | 0.12          |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 24       | 0.12          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 27       | 0.12          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 27       | 0.12          |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 27       | 0.12          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 30       | 0.12          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 30       | 0.12          |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 30       | 0.12          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 34       | 0.12          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 34       | 0.12          |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 34       | 0.12          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 39       | 0.12          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 39       | 0.12          |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 39       | 0.12          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 12       | 0.12          |
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 12       | 0.12          |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 12       | 0.12          |
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 18       | 0.12          |
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 18       | 0.12          |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 18       | 0.12          |
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 21       | 0.12          |
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 21       | 0.12          |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 21       | 0.12          |
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 24       | 0.12          |
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 24       | 0.12          |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 24       | 0.12          |
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 26       | 0.12          |
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 26       | 0.12          |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 26       | 0.12          |
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 27       | 0.12          |
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 27       | 0.12          |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 27       | 0.12          |
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 37       | 0.12          |
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 37       | 0.12          |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 37       | 0.12          |
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 38       | 0.12          |
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 38       | 0.12          |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 38       | 0.12          |
| (3,1899) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3 | 4        | 0.12          |
| (3,1899) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3 | 4        | 0.12          |
| (3,1899) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3 | 4        | 0.12          |
| (3,1899) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3 | 8        | 0.12          |
| (3,1899) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3 | 8        | 0.12          |
| (3,1899) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3 | 8        | 0.12          |
| (3,1899) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3 | 11       | 0.12          |
| (3,1899) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3 | 11       | 0.12          |
| (3,1899) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3 | 11       | 0.12          |
| (3,1899) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3 | 38       | 0.12          |
| (3,1899) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3 | 38       | 0.12          |
| (3,1899) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3 | 38       | 0.12          |
| (3,1885) | 1:23:A:GLU:HG3  | 1:72:A:THR:HA  | 29       | 0.12          |
| (3,1864) | 1:7:A:ALA:HB1   | 1:88:A:ARG:HA  | 3        | 0.12          |
| (3,1864) | 1:7:A:ALA:HB2   | 1:88:A:ARG:HA  | 3        | 0.12          |
| (3,1864) | 1:7:A:ALA:HB3   | 1:88:A:ARG:HA  | 3        | 0.12          |
| (3,1856) | 1:27:A:ALA:HB1  | 1:28:A:THR:H   | 9        | 0.12          |
| (3,1856) | 1:27:A:ALA:HB2  | 1:28:A:THR:H   | 9        | 0.12          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,1856) | 1:27:A:ALA:HB3 | 1:28:A:THR:H    | 9        | 0.12          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 1        | 0.12          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 9        | 0.12          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 11       | 0.12          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 16       | 0.12          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 17       | 0.12          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 22       | 0.12          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 25       | 0.12          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 31       | 0.12          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 37       | 0.12          |
| (3,1806) | 1:98:A:LYS:HG2 | 1:98:A:LYS:HB3  | 38       | 0.12          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG11 | 3        | 0.12          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG12 | 3        | 0.12          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG13 | 3        | 0.12          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG11 | 3        | 0.12          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG12 | 3        | 0.12          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG13 | 3        | 0.12          |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG11 | 3        | 0.12          |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG12 | 3        | 0.12          |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG13 | 3        | 0.12          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG11 | 8        | 0.12          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG12 | 8        | 0.12          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG13 | 8        | 0.12          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG11 | 8        | 0.12          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG12 | 8        | 0.12          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG13 | 8        | 0.12          |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG11 | 8        | 0.12          |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG12 | 8        | 0.12          |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG13 | 8        | 0.12          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG11 | 12       | 0.12          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG12 | 12       | 0.12          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG13 | 12       | 0.12          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG11 | 12       | 0.12          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG12 | 12       | 0.12          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG13 | 12       | 0.12          |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG11 | 12       | 0.12          |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG12 | 12       | 0.12          |
| (3,1721) | 1:38:A:ALA:HB3 | 1:33:A:VAL:HG13 | 12       | 0.12          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG11 | 23       | 0.12          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG12 | 23       | 0.12          |
| (3,1721) | 1:38:A:ALA:HB1 | 1:33:A:VAL:HG13 | 23       | 0.12          |
| (3,1721) | 1:38:A:ALA:HB2 | 1:33:A:VAL:HG11 | 23       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG12 | 23       | 0.12          |
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 23       | 0.12          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 23       | 0.12          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 23       | 0.12          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 23       | 0.12          |
| (3,1721) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG11 | 37       | 0.12          |
| (3,1721) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG12 | 37       | 0.12          |
| (3,1721) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG13 | 37       | 0.12          |
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG11 | 37       | 0.12          |
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG12 | 37       | 0.12          |
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 37       | 0.12          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 37       | 0.12          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 37       | 0.12          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 37       | 0.12          |
| (3,1712) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 1        | 0.12          |
| (3,1712) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 1        | 0.12          |
| (3,1712) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 1        | 0.12          |
| (3,1712) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 2        | 0.12          |
| (3,1712) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 2        | 0.12          |
| (3,1712) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 2        | 0.12          |
| (3,1712) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 5        | 0.12          |
| (3,1712) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 5        | 0.12          |
| (3,1712) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 5        | 0.12          |
| (3,1712) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 20       | 0.12          |
| (3,1712) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 20       | 0.12          |
| (3,1712) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 20       | 0.12          |
| (3,1712) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 25       | 0.12          |
| (3,1712) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 25       | 0.12          |
| (3,1712) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 25       | 0.12          |
| (3,1712) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 27       | 0.12          |
| (3,1712) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 27       | 0.12          |
| (3,1712) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 27       | 0.12          |
| (3,1712) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 36       | 0.12          |
| (3,1712) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 36       | 0.12          |
| (3,1712) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 36       | 0.12          |
| (3,1712) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 37       | 0.12          |
| (3,1712) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 37       | 0.12          |
| (3,1712) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 37       | 0.12          |
| (3,1712) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 38       | 0.12          |
| (3,1712) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 38       | 0.12          |
| (3,1712) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 38       | 0.12          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 12       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 12       | 0.12          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 12       | 0.12          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 12       | 0.12          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 12       | 0.12          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 12       | 0.12          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 12       | 0.12          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 12       | 0.12          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 12       | 0.12          |
| (3,1683) | 1:85:A:LEU:HD11 | 1:35:A:PHE:HD1  | 4        | 0.12          |
| (3,1683) | 1:85:A:LEU:HD11 | 1:35:A:PHE:HD2  | 4        | 0.12          |
| (3,1683) | 1:85:A:LEU:HD12 | 1:35:A:PHE:HD1  | 4        | 0.12          |
| (3,1683) | 1:85:A:LEU:HD12 | 1:35:A:PHE:HD2  | 4        | 0.12          |
| (3,1683) | 1:85:A:LEU:HD13 | 1:35:A:PHE:HD1  | 4        | 0.12          |
| (3,1683) | 1:85:A:LEU:HD13 | 1:35:A:PHE:HD2  | 4        | 0.12          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 27       | 0.12          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 27       | 0.12          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 27       | 0.12          |
| (3,1657) | 1:81:A:VAL:HG11 | 1:31:A:CYS:HB2  | 5        | 0.12          |
| (3,1657) | 1:81:A:VAL:HG12 | 1:31:A:CYS:HB2  | 5        | 0.12          |
| (3,1657) | 1:81:A:VAL:HG13 | 1:31:A:CYS:HB2  | 5        | 0.12          |
| (3,1654) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 28       | 0.12          |
| (3,1654) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 28       | 0.12          |
| (3,1654) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 28       | 0.12          |
| (3,1654) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 28       | 0.12          |
| (3,1654) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 28       | 0.12          |
| (3,1654) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 28       | 0.12          |
| (3,1654) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 28       | 0.12          |
| (3,1654) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 28       | 0.12          |
| (3,1654) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 28       | 0.12          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 20       | 0.12          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 20       | 0.12          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 20       | 0.12          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 20       | 0.12          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 20       | 0.12          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 20       | 0.12          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 20       | 0.12          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 20       | 0.12          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 20       | 0.12          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 3        | 0.12          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 3        | 0.12          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 3        | 0.12          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 7        | 0.12          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H   | 7        | 0.12          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 7        | 0.12          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H   | 12       | 0.12          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H   | 12       | 0.12          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 12       | 0.12          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H   | 20       | 0.12          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H   | 20       | 0.12          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 20       | 0.12          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H   | 26       | 0.12          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H   | 26       | 0.12          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 26       | 0.12          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H   | 33       | 0.12          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H   | 33       | 0.12          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 33       | 0.12          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H   | 36       | 0.12          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H   | 36       | 0.12          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 36       | 0.12          |
| (3,1631) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H   | 37       | 0.12          |
| (3,1631) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H   | 37       | 0.12          |
| (3,1631) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 37       | 0.12          |
| (3,1628) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2 | 2        | 0.12          |
| (3,1628) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2 | 2        | 0.12          |
| (3,1628) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2 | 2        | 0.12          |
| (3,1626) | 1:82:A:ILE:HD11 | 1:83:A:ALA:H   | 8        | 0.12          |
| (3,1626) | 1:82:A:ILE:HD12 | 1:83:A:ALA:H   | 8        | 0.12          |
| (3,1626) | 1:82:A:ILE:HD13 | 1:83:A:ALA:H   | 8        | 0.12          |
| (3,1626) | 1:82:A:ILE:HD11 | 1:83:A:ALA:H   | 29       | 0.12          |
| (3,1626) | 1:82:A:ILE:HD12 | 1:83:A:ALA:H   | 29       | 0.12          |
| (3,1626) | 1:82:A:ILE:HD13 | 1:83:A:ALA:H   | 29       | 0.12          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2 | 13       | 0.12          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 13       | 0.12          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 13       | 0.12          |
| (3,1622) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2 | 28       | 0.12          |
| (3,1622) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 28       | 0.12          |
| (3,1622) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 28       | 0.12          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 8        | 0.12          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 8        | 0.12          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 8        | 0.12          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 8        | 0.12          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 8        | 0.12          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 8        | 0.12          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 29       | 0.12          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 29       | 0.12          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 29       | 0.12          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 29       | 0.12          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 29       | 0.12          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 29       | 0.12          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 33       | 0.12          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 33       | 0.12          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 33       | 0.12          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 33       | 0.12          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 33       | 0.12          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 33       | 0.12          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 1        | 0.12          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 1        | 0.12          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 1        | 0.12          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 1        | 0.12          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 1        | 0.12          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 1        | 0.12          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 4        | 0.12          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 4        | 0.12          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 4        | 0.12          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 4        | 0.12          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 4        | 0.12          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 4        | 0.12          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 14       | 0.12          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 14       | 0.12          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 14       | 0.12          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 14       | 0.12          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 14       | 0.12          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 14       | 0.12          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 32       | 0.12          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 32       | 0.12          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 32       | 0.12          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 32       | 0.12          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 32       | 0.12          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 32       | 0.12          |
| (3,1554) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA   | 11       | 0.12          |
| (3,1554) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA   | 11       | 0.12          |
| (3,1554) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA   | 11       | 0.12          |
| (3,1554) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA   | 22       | 0.12          |
| (3,1554) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA   | 22       | 0.12          |
| (3,1554) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA   | 22       | 0.12          |
| (3,1554) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA   | 34       | 0.12          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1554) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA   | 34       | 0.12          |
| (3,1554) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA   | 34       | 0.12          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 6        | 0.12          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 6        | 0.12          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 6        | 0.12          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 26       | 0.12          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 26       | 0.12          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 26       | 0.12          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 29       | 0.12          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 29       | 0.12          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 29       | 0.12          |
| (3,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 40       | 0.12          |
| (3,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 40       | 0.12          |
| (3,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 40       | 0.12          |
| (3,1517) | 1:66:A:MET:HE1  | 1:29:A:PHE:H   | 3        | 0.12          |
| (3,1517) | 1:66:A:MET:HE2  | 1:29:A:PHE:H   | 3        | 0.12          |
| (3,1517) | 1:66:A:MET:HE3  | 1:29:A:PHE:H   | 3        | 0.12          |
| (3,1517) | 1:66:A:MET:HE1  | 1:29:A:PHE:H   | 18       | 0.12          |
| (3,1517) | 1:66:A:MET:HE2  | 1:29:A:PHE:H   | 18       | 0.12          |
| (3,1517) | 1:66:A:MET:HE3  | 1:29:A:PHE:H   | 18       | 0.12          |
| (3,1517) | 1:66:A:MET:HE1  | 1:29:A:PHE:H   | 32       | 0.12          |
| (3,1517) | 1:66:A:MET:HE2  | 1:29:A:PHE:H   | 32       | 0.12          |
| (3,1517) | 1:66:A:MET:HE3  | 1:29:A:PHE:H   | 32       | 0.12          |
| (3,1517) | 1:66:A:MET:HE1  | 1:29:A:PHE:H   | 34       | 0.12          |
| (3,1517) | 1:66:A:MET:HE2  | 1:29:A:PHE:H   | 34       | 0.12          |
| (3,1517) | 1:66:A:MET:HE3  | 1:29:A:PHE:H   | 34       | 0.12          |
| (3,1514) | 1:66:A:MET:HE1  | 1:42:A:TRP:HE1 | 7        | 0.12          |
| (3,1514) | 1:66:A:MET:HE2  | 1:42:A:TRP:HE1 | 7        | 0.12          |
| (3,1514) | 1:66:A:MET:HE3  | 1:42:A:TRP:HE1 | 7        | 0.12          |
| (3,1514) | 1:66:A:MET:HE1  | 1:42:A:TRP:HE1 | 10       | 0.12          |
| (3,1514) | 1:66:A:MET:HE2  | 1:42:A:TRP:HE1 | 10       | 0.12          |
| (3,1514) | 1:66:A:MET:HE3  | 1:42:A:TRP:HE1 | 10       | 0.12          |
| (3,1514) | 1:66:A:MET:HE1  | 1:42:A:TRP:HE1 | 34       | 0.12          |
| (3,1514) | 1:66:A:MET:HE2  | 1:42:A:TRP:HE1 | 34       | 0.12          |
| (3,1514) | 1:66:A:MET:HE3  | 1:42:A:TRP:HE1 | 34       | 0.12          |
| (3,1514) | 1:66:A:MET:HE1  | 1:42:A:TRP:HE1 | 38       | 0.12          |
| (3,1514) | 1:66:A:MET:HE2  | 1:42:A:TRP:HE1 | 38       | 0.12          |
| (3,1514) | 1:66:A:MET:HE3  | 1:42:A:TRP:HE1 | 38       | 0.12          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1 | 6        | 0.12          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2 | 6        | 0.12          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1 | 6        | 0.12          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2 | 6        | 0.12          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 6        | 0.12          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 6        | 0.12          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 15       | 0.12          |
| (3,1513) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 15       | 0.12          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 15       | 0.12          |
| (3,1513) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 15       | 0.12          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 15       | 0.12          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 15       | 0.12          |
| (3,1512) | 1:66:A:MET:HE1 | 1:42:A:TRP:HZ3 | 3        | 0.12          |
| (3,1512) | 1:66:A:MET:HE2 | 1:42:A:TRP:HZ3 | 3        | 0.12          |
| (3,1512) | 1:66:A:MET:HE3 | 1:42:A:TRP:HZ3 | 3        | 0.12          |
| (3,1512) | 1:66:A:MET:HE1 | 1:42:A:TRP:HZ3 | 26       | 0.12          |
| (3,1512) | 1:66:A:MET:HE2 | 1:42:A:TRP:HZ3 | 26       | 0.12          |
| (3,1512) | 1:66:A:MET:HE3 | 1:42:A:TRP:HZ3 | 26       | 0.12          |
| (3,1512) | 1:66:A:MET:HE1 | 1:42:A:TRP:HZ3 | 31       | 0.12          |
| (3,1512) | 1:66:A:MET:HE2 | 1:42:A:TRP:HZ3 | 31       | 0.12          |
| (3,1512) | 1:66:A:MET:HE3 | 1:42:A:TRP:HZ3 | 31       | 0.12          |
| (3,1512) | 1:66:A:MET:HE1 | 1:42:A:TRP:HZ3 | 32       | 0.12          |
| (3,1512) | 1:66:A:MET:HE2 | 1:42:A:TRP:HZ3 | 32       | 0.12          |
| (3,1512) | 1:66:A:MET:HE3 | 1:42:A:TRP:HZ3 | 32       | 0.12          |
| (3,1511) | 1:66:A:MET:HE1 | 1:42:A:TRP:HB2 | 14       | 0.12          |
| (3,1511) | 1:66:A:MET:HE2 | 1:42:A:TRP:HB2 | 14       | 0.12          |
| (3,1511) | 1:66:A:MET:HE3 | 1:42:A:TRP:HB2 | 14       | 0.12          |
| (3,1511) | 1:66:A:MET:HE1 | 1:42:A:TRP:HB2 | 32       | 0.12          |
| (3,1511) | 1:66:A:MET:HE2 | 1:42:A:TRP:HB2 | 32       | 0.12          |
| (3,1511) | 1:66:A:MET:HE3 | 1:42:A:TRP:HB2 | 32       | 0.12          |
| (3,1511) | 1:66:A:MET:HE1 | 1:42:A:TRP:HB2 | 34       | 0.12          |
| (3,1511) | 1:66:A:MET:HE2 | 1:42:A:TRP:HB2 | 34       | 0.12          |
| (3,1511) | 1:66:A:MET:HE3 | 1:42:A:TRP:HB2 | 34       | 0.12          |
| (3,1507) | 1:66:A:MET:HE1 | 1:66:A:MET:HG2 | 2        | 0.12          |
| (3,1507) | 1:66:A:MET:HE2 | 1:66:A:MET:HG2 | 2        | 0.12          |
| (3,1507) | 1:66:A:MET:HE3 | 1:66:A:MET:HG2 | 2        | 0.12          |
| (3,1507) | 1:66:A:MET:HE1 | 1:66:A:MET:HG2 | 6        | 0.12          |
| (3,1507) | 1:66:A:MET:HE2 | 1:66:A:MET:HG2 | 6        | 0.12          |
| (3,1507) | 1:66:A:MET:HE3 | 1:66:A:MET:HG2 | 6        | 0.12          |
| (3,1507) | 1:66:A:MET:HE1 | 1:66:A:MET:HG2 | 7        | 0.12          |
| (3,1507) | 1:66:A:MET:HE2 | 1:66:A:MET:HG2 | 7        | 0.12          |
| (3,1507) | 1:66:A:MET:HE3 | 1:66:A:MET:HG2 | 7        | 0.12          |
| (3,1507) | 1:66:A:MET:HE1 | 1:66:A:MET:HG2 | 10       | 0.12          |
| (3,1507) | 1:66:A:MET:HE2 | 1:66:A:MET:HG2 | 10       | 0.12          |
| (3,1507) | 1:66:A:MET:HE3 | 1:66:A:MET:HG2 | 10       | 0.12          |
| (3,1507) | 1:66:A:MET:HE1 | 1:66:A:MET:HG2 | 12       | 0.12          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1507) | 1:66:A:MET:HE2  | 1:66:A:MET:HG2 | 12       | 0.12          |
| (3,1507) | 1:66:A:MET:HE3  | 1:66:A:MET:HG2 | 12       | 0.12          |
| (3,1507) | 1:66:A:MET:HE1  | 1:66:A:MET:HG2 | 21       | 0.12          |
| (3,1507) | 1:66:A:MET:HE2  | 1:66:A:MET:HG2 | 21       | 0.12          |
| (3,1507) | 1:66:A:MET:HE3  | 1:66:A:MET:HG2 | 21       | 0.12          |
| (3,1507) | 1:66:A:MET:HE1  | 1:66:A:MET:HG2 | 24       | 0.12          |
| (3,1507) | 1:66:A:MET:HE2  | 1:66:A:MET:HG2 | 24       | 0.12          |
| (3,1507) | 1:66:A:MET:HE3  | 1:66:A:MET:HG2 | 24       | 0.12          |
| (3,1507) | 1:66:A:MET:HE1  | 1:66:A:MET:HG2 | 28       | 0.12          |
| (3,1507) | 1:66:A:MET:HE2  | 1:66:A:MET:HG2 | 28       | 0.12          |
| (3,1507) | 1:66:A:MET:HE3  | 1:66:A:MET:HG2 | 28       | 0.12          |
| (3,1507) | 1:66:A:MET:HE1  | 1:66:A:MET:HG2 | 40       | 0.12          |
| (3,1507) | 1:66:A:MET:HE2  | 1:66:A:MET:HG2 | 40       | 0.12          |
| (3,1507) | 1:66:A:MET:HE3  | 1:66:A:MET:HG2 | 40       | 0.12          |
| (3,1498) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ  | 1        | 0.12          |
| (3,1498) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ  | 1        | 0.12          |
| (3,1498) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ  | 1        | 0.12          |
| (3,1498) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ  | 8        | 0.12          |
| (3,1498) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ  | 8        | 0.12          |
| (3,1498) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ  | 8        | 0.12          |
| (3,1498) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ  | 16       | 0.12          |
| (3,1498) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ  | 16       | 0.12          |
| (3,1498) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ  | 16       | 0.12          |
| (3,1498) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ  | 18       | 0.12          |
| (3,1498) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ  | 18       | 0.12          |
| (3,1498) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ  | 18       | 0.12          |
| (3,1498) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ  | 21       | 0.12          |
| (3,1498) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ  | 21       | 0.12          |
| (3,1498) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ  | 21       | 0.12          |
| (3,1498) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ  | 26       | 0.12          |
| (3,1498) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ  | 26       | 0.12          |
| (3,1498) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ  | 26       | 0.12          |
| (3,1498) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ  | 28       | 0.12          |
| (3,1498) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ  | 28       | 0.12          |
| (3,1498) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ  | 28       | 0.12          |
| (3,1498) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ  | 35       | 0.12          |
| (3,1498) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ  | 35       | 0.12          |
| (3,1498) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ  | 35       | 0.12          |
| (3,1498) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ  | 36       | 0.12          |
| (3,1498) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ  | 36       | 0.12          |
| (3,1498) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ  | 36       | 0.12          |
| (3,1498) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ  | 37       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1498) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 37       | 0.12          |
| (3,1498) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 37       | 0.12          |
| (3,1498) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 40       | 0.12          |
| (3,1498) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 40       | 0.12          |
| (3,1498) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 40       | 0.12          |
| (3,1488) | 1:81:A:VAL:HB   | 1:42:A:TRP:HE1  | 17       | 0.12          |
| (3,1488) | 1:81:A:VAL:HB   | 1:42:A:TRP:HE1  | 18       | 0.12          |
| (3,1488) | 1:81:A:VAL:HB   | 1:42:A:TRP:HE1  | 20       | 0.12          |
| (3,1424) | 1:21:A:VAL:HG21 | 1:19:A:ILE:HD11 | 5        | 0.12          |
| (3,1424) | 1:21:A:VAL:HG21 | 1:19:A:ILE:HD12 | 5        | 0.12          |
| (3,1424) | 1:21:A:VAL:HG21 | 1:19:A:ILE:HD13 | 5        | 0.12          |
| (3,1424) | 1:21:A:VAL:HG22 | 1:19:A:ILE:HD11 | 5        | 0.12          |
| (3,1424) | 1:21:A:VAL:HG22 | 1:19:A:ILE:HD12 | 5        | 0.12          |
| (3,1424) | 1:21:A:VAL:HG22 | 1:19:A:ILE:HD13 | 5        | 0.12          |
| (3,1424) | 1:21:A:VAL:HG23 | 1:19:A:ILE:HD11 | 5        | 0.12          |
| (3,1424) | 1:21:A:VAL:HG23 | 1:19:A:ILE:HD12 | 5        | 0.12          |
| (3,1424) | 1:21:A:VAL:HG23 | 1:19:A:ILE:HD13 | 5        | 0.12          |
| (3,1412) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HA  | 6        | 0.12          |
| (3,1412) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HA  | 6        | 0.12          |
| (3,1412) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HA  | 6        | 0.12          |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H    | 8        | 0.12          |
| (3,1407) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H    | 8        | 0.12          |
| (3,1407) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H    | 8        | 0.12          |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H    | 22       | 0.12          |
| (3,1407) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H    | 22       | 0.12          |
| (3,1407) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H    | 22       | 0.12          |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H    | 26       | 0.12          |
| (3,1407) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H    | 26       | 0.12          |
| (3,1407) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H    | 26       | 0.12          |
| (3,1405) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H    | 28       | 0.12          |
| (3,1405) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H    | 28       | 0.12          |
| (3,1405) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H    | 28       | 0.12          |
| (3,1404) | 1:95:A:ALA:HB1  | 1:16:A:ILE:HG12 | 19       | 0.12          |
| (3,1404) | 1:95:A:ALA:HB2  | 1:16:A:ILE:HG12 | 19       | 0.12          |
| (3,1404) | 1:95:A:ALA:HB3  | 1:16:A:ILE:HG12 | 19       | 0.12          |
| (3,1404) | 1:95:A:ALA:HB1  | 1:16:A:ILE:HG12 | 30       | 0.12          |
| (3,1404) | 1:95:A:ALA:HB2  | 1:16:A:ILE:HG12 | 30       | 0.12          |
| (3,1404) | 1:95:A:ALA:HB3  | 1:16:A:ILE:HG12 | 30       | 0.12          |
| (3,1391) | 1:91:A:ALA:HB1  | 1:12:A:PHE:HZ   | 12       | 0.12          |
| (3,1391) | 1:91:A:ALA:HB2  | 1:12:A:PHE:HZ   | 12       | 0.12          |
| (3,1391) | 1:91:A:ALA:HB3  | 1:12:A:PHE:HZ   | 12       | 0.12          |
| (3,1391) | 1:91:A:ALA:HB1  | 1:12:A:PHE:HZ   | 19       | 0.12          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,1391) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ  | 19       | 0.12          |
| (3,1391) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ  | 19       | 0.12          |
| (3,1391) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ  | 24       | 0.12          |
| (3,1391) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ  | 24       | 0.12          |
| (3,1391) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ  | 24       | 0.12          |
| (3,1391) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ  | 25       | 0.12          |
| (3,1391) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ  | 25       | 0.12          |
| (3,1391) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ  | 25       | 0.12          |
| (3,1391) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ  | 40       | 0.12          |
| (3,1391) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ  | 40       | 0.12          |
| (3,1391) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ  | 40       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 4        | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 4        | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 4        | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 4        | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 4        | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 4        | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 4        | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 4        | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 4        | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 8        | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 8        | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 8        | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 8        | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 8        | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 8        | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 8        | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 8        | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 8        | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 10       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 10       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 10       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 10       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 10       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 10       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 10       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 10       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 10       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 12       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 12       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 12       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 12       | 0.12          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 12       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 12       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 12       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 12       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 12       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 17       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 17       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 17       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 17       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 17       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 17       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 17       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 17       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 17       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 21       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 21       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 21       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 21       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 21       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 21       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 21       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 21       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 21       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 23       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 23       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 23       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 23       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 23       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 23       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 23       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 23       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 23       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 27       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 27       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 27       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 27       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 27       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 27       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 27       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 27       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 27       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 28       | 0.12          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 28       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 28       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 28       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 28       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 28       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 28       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 28       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 28       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 29       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 29       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 29       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 29       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 29       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 29       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 29       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 29       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 29       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 32       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 32       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 32       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 32       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 32       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 32       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 32       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 32       | 0.12          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 32       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 4        | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 4        | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 4        | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 4        | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 4        | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 4        | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 4        | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 4        | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 4        | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 8        | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 8        | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 8        | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 8        | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 8        | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 8        | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 8        | 0.12          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 8        | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 8        | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 10       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 10       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 10       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 10       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 10       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 10       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 10       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 10       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 10       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 12       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 12       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 12       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 12       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 12       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 12       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 12       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 12       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 12       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 17       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 17       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 17       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 17       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 17       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 17       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 17       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 17       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 17       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 21       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 21       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 21       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 21       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 21       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 21       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 21       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 21       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 21       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 23       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 23       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 23       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 23       | 0.12          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 23       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 23       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 23       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 23       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 23       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 27       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 27       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 27       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 27       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 27       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 27       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 27       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 27       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 27       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 28       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 28       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 28       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 28       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 28       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 28       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 28       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 28       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 28       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 29       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 29       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 29       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 29       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 29       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 29       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 29       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 29       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 29       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 32       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 32       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 32       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 32       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 32       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 32       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 32       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 32       | 0.12          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 32       | 0.12          |
| (3,1372) | 1:16:A:ILE:HB  | 1:29:A:PHE:HB3 | 7        | 0.12          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3 | 24       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA  | 2        | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA  | 2        | 0.12          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA  | 2        | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA  | 4        | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA  | 4        | 0.12          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA  | 4        | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA  | 5        | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA  | 5        | 0.12          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA  | 5        | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA  | 7        | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA  | 7        | 0.12          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA  | 7        | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA  | 8        | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA  | 8        | 0.12          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA  | 8        | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA  | 9        | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA  | 9        | 0.12          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA  | 9        | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA  | 10       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA  | 10       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA  | 10       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA  | 11       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA  | 11       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA  | 11       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA  | 12       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA  | 12       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA  | 12       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA  | 13       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA  | 13       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA  | 13       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA  | 16       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA  | 16       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA  | 16       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA  | 17       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA  | 17       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA  | 17       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA  | 18       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA  | 18       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA  | 18       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA  | 21       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA  | 21       | 0.12          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 21       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 22       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 22       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 22       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 24       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 24       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 24       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 25       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 25       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 25       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 26       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 26       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 26       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 27       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 27       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 27       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 29       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 29       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 29       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 30       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 30       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 30       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 31       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 31       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 31       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 32       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 32       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 32       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 33       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 33       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 33       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 34       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 34       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 34       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 35       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 35       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 35       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 36       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 36       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 36       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 37       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 37       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA   | 37       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA   | 38       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA   | 38       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA   | 38       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA   | 39       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA   | 39       | 0.12          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA   | 39       | 0.12          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 18       | 0.12          |
| (3,1329) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 34       | 0.12          |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 6        | 0.12          |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 12       | 0.12          |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 13       | 0.12          |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 16       | 0.12          |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 19       | 0.12          |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 23       | 0.12          |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 26       | 0.12          |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 31       | 0.12          |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 40       | 0.12          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 20       | 0.12          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 20       | 0.12          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 20       | 0.12          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 30       | 0.12          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 30       | 0.12          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 30       | 0.12          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1  | 6        | 0.12          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2  | 6        | 0.12          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3  | 6        | 0.12          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1  | 6        | 0.12          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2  | 6        | 0.12          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3  | 6        | 0.12          |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1  | 6        | 0.12          |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2  | 6        | 0.12          |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3  | 6        | 0.12          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1  | 23       | 0.12          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2  | 23       | 0.12          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3  | 23       | 0.12          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1  | 23       | 0.12          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2  | 23       | 0.12          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3  | 23       | 0.12          |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1  | 23       | 0.12          |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2  | 23       | 0.12          |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3  | 23       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1293) | 1:40:A:VAL:HG21 | 1:42:A:TRP:HE1  | 29       | 0.12          |
| (3,1293) | 1:40:A:VAL:HG22 | 1:42:A:TRP:HE1  | 29       | 0.12          |
| (3,1293) | 1:40:A:VAL:HG23 | 1:42:A:TRP:HE1  | 29       | 0.12          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 20       | 0.12          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 20       | 0.12          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 20       | 0.12          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 30       | 0.12          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 30       | 0.12          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 30       | 0.12          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3   | 16       | 0.12          |
| (3,1274) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3   | 33       | 0.12          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 16       | 0.12          |
| (3,1273) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 33       | 0.12          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 12       | 0.12          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 12       | 0.12          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 12       | 0.12          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 12       | 0.12          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 12       | 0.12          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 12       | 0.12          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 12       | 0.12          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 12       | 0.12          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 12       | 0.12          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 23       | 0.12          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 23       | 0.12          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 23       | 0.12          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 23       | 0.12          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 23       | 0.12          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 23       | 0.12          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 23       | 0.12          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 23       | 0.12          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 23       | 0.12          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 33       | 0.12          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 33       | 0.12          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 33       | 0.12          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 33       | 0.12          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 33       | 0.12          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 33       | 0.12          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 33       | 0.12          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 33       | 0.12          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 33       | 0.12          |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 17       | 0.12          |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 17       | 0.12          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H  | 17       | 0.12          |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H  | 17       | 0.12          |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H  | 17       | 0.12          |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H  | 17       | 0.12          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA | 1        | 0.12          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA | 1        | 0.12          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA | 1        | 0.12          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA | 5        | 0.12          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA | 5        | 0.12          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA | 5        | 0.12          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA | 8        | 0.12          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA | 8        | 0.12          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA | 8        | 0.12          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA | 15       | 0.12          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA | 15       | 0.12          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA | 15       | 0.12          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA | 18       | 0.12          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA | 18       | 0.12          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA | 18       | 0.12          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA | 22       | 0.12          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA | 22       | 0.12          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA | 22       | 0.12          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA | 27       | 0.12          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA | 27       | 0.12          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA | 27       | 0.12          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA | 39       | 0.12          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA | 39       | 0.12          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA | 39       | 0.12          |
| (3,1265) | 1:67:A:THR:HG21 | 1:56:A:ASN:H  | 14       | 0.12          |
| (3,1265) | 1:67:A:THR:HG22 | 1:56:A:ASN:H  | 14       | 0.12          |
| (3,1265) | 1:67:A:THR:HG23 | 1:56:A:ASN:H  | 14       | 0.12          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H  | 12       | 0.12          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H  | 12       | 0.12          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H  | 12       | 0.12          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H  | 22       | 0.12          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H  | 22       | 0.12          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H  | 22       | 0.12          |
| (3,1243) | 1:13:A:THR:HG21 | 1:34:A:SER:H  | 3        | 0.12          |
| (3,1243) | 1:13:A:THR:HG22 | 1:34:A:SER:H  | 3        | 0.12          |
| (3,1243) | 1:13:A:THR:HG23 | 1:34:A:SER:H  | 3        | 0.12          |
| (3,1243) | 1:13:A:THR:HG21 | 1:34:A:SER:H  | 28       | 0.12          |
| (3,1243) | 1:13:A:THR:HG22 | 1:34:A:SER:H  | 28       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1243) | 1:13:A:THR:HG23 | 1:34:A:SER:H    | 28       | 0.12          |
| (3,1243) | 1:13:A:THR:HG21 | 1:34:A:SER:H    | 39       | 0.12          |
| (3,1243) | 1:13:A:THR:HG22 | 1:34:A:SER:H    | 39       | 0.12          |
| (3,1243) | 1:13:A:THR:HG23 | 1:34:A:SER:H    | 39       | 0.12          |
| (3,1240) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3  | 22       | 0.12          |
| (3,1240) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3  | 22       | 0.12          |
| (3,1240) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3  | 22       | 0.12          |
| (3,1240) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3  | 31       | 0.12          |
| (3,1240) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3  | 31       | 0.12          |
| (3,1240) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3  | 31       | 0.12          |
| (3,1232) | 1:89:A:GLY:H    | 1:9:A:PRO:HG3   | 26       | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 1        | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 1        | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 1        | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 4        | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 4        | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 4        | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 7        | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 7        | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 7        | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 11       | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 11       | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 11       | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 17       | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 17       | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 17       | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 23       | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 23       | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 23       | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 25       | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 25       | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 25       | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 29       | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 29       | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 29       | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 37       | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 37       | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 37       | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 39       | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 39       | 0.12          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 39       | 0.12          |
| (3,1217) | 1:66:A:MET:H    | 1:28:A:THR:HA   | 6        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1212) | 1:56:A:ASN:H    | 1:66:A:MET:HG2  | 1        | 0.12          |
| (3,1208) | 1:42:A:TRP:H    | 1:57:A:PHE:HE1  | 12       | 0.12          |
| (3,1208) | 1:42:A:TRP:H    | 1:57:A:PHE:HE2  | 12       | 0.12          |
| (3,1208) | 1:42:A:TRP:H    | 1:57:A:PHE:HE1  | 19       | 0.12          |
| (3,1208) | 1:42:A:TRP:H    | 1:57:A:PHE:HE2  | 19       | 0.12          |
| (3,1180) | 1:47:A:THR:H    | 1:44:A:LYS:HB3  | 14       | 0.12          |
| (3,1180) | 1:47:A:THR:H    | 1:44:A:LYS:HB3  | 15       | 0.12          |
| (3,1180) | 1:47:A:THR:H    | 1:44:A:LYS:HB3  | 16       | 0.12          |
| (3,1180) | 1:47:A:THR:H    | 1:44:A:LYS:HB3  | 23       | 0.12          |
| (3,1180) | 1:47:A:THR:H    | 1:44:A:LYS:HB3  | 39       | 0.12          |
| (3,1178) | 1:91:A:ALA:H    | 1:84:A:ARG:HA   | 35       | 0.12          |
| (3,1167) | 1:75:A:ASP:H    | 1:74:A:ASP:HB2  | 28       | 0.12          |
| (3,1152) | 1:54:A:LYS:H    | 1:53:A:GLN:HG3  | 20       | 0.12          |
| (3,1152) | 1:54:A:LYS:H    | 1:53:A:GLN:HG3  | 33       | 0.12          |
| (3,1140) | 1:100:A:GLU:H   | 1:101:A:LEU:H   | 39       | 0.12          |
| (3,1096) | 1:74:A:ASP:H    | 1:73:A:PRO:HA   | 21       | 0.12          |
| (3,1096) | 1:74:A:ASP:H    | 1:73:A:PRO:HA   | 23       | 0.12          |
| (3,1096) | 1:74:A:ASP:H    | 1:73:A:PRO:HA   | 24       | 0.12          |
| (3,1096) | 1:74:A:ASP:H    | 1:73:A:PRO:HA   | 27       | 0.12          |
| (3,1096) | 1:74:A:ASP:H    | 1:73:A:PRO:HA   | 29       | 0.12          |
| (3,1096) | 1:74:A:ASP:H    | 1:73:A:PRO:HA   | 33       | 0.12          |
| (3,1096) | 1:74:A:ASP:H    | 1:73:A:PRO:HA   | 40       | 0.12          |
| (3,1063) | 1:71:A:VAL:H    | 1:25:A:GLN:H    | 18       | 0.12          |
| (3,1063) | 1:71:A:VAL:H    | 1:25:A:GLN:H    | 39       | 0.12          |
| (3,1051) | 1:26:A:SER:H    | 1:25:A:GLN:HG2  | 11       | 0.12          |
| (3,1051) | 1:26:A:SER:H    | 1:25:A:GLN:HG2  | 14       | 0.12          |
| (3,1051) | 1:26:A:SER:H    | 1:25:A:GLN:HG2  | 15       | 0.12          |
| (3,1051) | 1:26:A:SER:H    | 1:25:A:GLN:HG2  | 25       | 0.12          |
| (3,1036) | 1:56:A:ASN:HD22 | 1:56:A:ASN:HA   | 32       | 0.12          |
| (3,1019) | 1:48:A:GLU:H    | 1:48:A:GLU:HG3  | 3        | 0.12          |
| (3,1019) | 1:48:A:GLU:H    | 1:48:A:GLU:HG3  | 7        | 0.12          |
| (3,1019) | 1:48:A:GLU:H    | 1:48:A:GLU:HG3  | 13       | 0.12          |
| (3,1019) | 1:48:A:GLU:H    | 1:48:A:GLU:HG3  | 24       | 0.12          |
| (3,1019) | 1:48:A:GLU:H    | 1:48:A:GLU:HG3  | 25       | 0.12          |
| (3,1019) | 1:48:A:GLU:H    | 1:48:A:GLU:HG3  | 32       | 0.12          |
| (3,1019) | 1:48:A:GLU:H    | 1:48:A:GLU:HG3  | 40       | 0.12          |
| (3,998)  | 1:79:A:TYR:H    | 1:94:A:THR:HG21 | 5        | 0.12          |
| (3,998)  | 1:79:A:TYR:H    | 1:94:A:THR:HG22 | 5        | 0.12          |
| (3,998)  | 1:79:A:TYR:H    | 1:94:A:THR:HG23 | 5        | 0.12          |
| (3,998)  | 1:79:A:TYR:H    | 1:94:A:THR:HG21 | 8        | 0.12          |
| (3,998)  | 1:79:A:TYR:H    | 1:94:A:THR:HG22 | 8        | 0.12          |
| (3,998)  | 1:79:A:TYR:H    | 1:94:A:THR:HG23 | 8        | 0.12          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,998) | 1:79:A:TYR:H | 1:94:A:THR:HG21 | 11       | 0.12          |
| (3,998) | 1:79:A:TYR:H | 1:94:A:THR:HG22 | 11       | 0.12          |
| (3,998) | 1:79:A:TYR:H | 1:94:A:THR:HG23 | 11       | 0.12          |
| (3,998) | 1:79:A:TYR:H | 1:94:A:THR:HG21 | 12       | 0.12          |
| (3,998) | 1:79:A:TYR:H | 1:94:A:THR:HG22 | 12       | 0.12          |
| (3,998) | 1:79:A:TYR:H | 1:94:A:THR:HG23 | 12       | 0.12          |
| (3,998) | 1:79:A:TYR:H | 1:94:A:THR:HG21 | 14       | 0.12          |
| (3,998) | 1:79:A:TYR:H | 1:94:A:THR:HG22 | 14       | 0.12          |
| (3,998) | 1:79:A:TYR:H | 1:94:A:THR:HG23 | 14       | 0.12          |
| (3,998) | 1:79:A:TYR:H | 1:94:A:THR:HG21 | 24       | 0.12          |
| (3,998) | 1:79:A:TYR:H | 1:94:A:THR:HG22 | 24       | 0.12          |
| (3,998) | 1:79:A:TYR:H | 1:94:A:THR:HG23 | 24       | 0.12          |
| (3,998) | 1:79:A:TYR:H | 1:94:A:THR:HG21 | 27       | 0.12          |
| (3,998) | 1:79:A:TYR:H | 1:94:A:THR:HG22 | 27       | 0.12          |
| (3,998) | 1:79:A:TYR:H | 1:94:A:THR:HG23 | 27       | 0.12          |
| (3,988) | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 11       | 0.12          |
| (3,988) | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 12       | 0.12          |
| (3,988) | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 26       | 0.12          |
| (3,988) | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 36       | 0.12          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 18       | 0.12          |
| (3,979) | 1:20:A:VAL:H | 1:19:A:ILE:HB   | 34       | 0.12          |
| (3,972) | 1:21:A:VAL:H | 1:21:A:VAL:HG21 | 7        | 0.12          |
| (3,972) | 1:21:A:VAL:H | 1:21:A:VAL:HG22 | 7        | 0.12          |
| (3,972) | 1:21:A:VAL:H | 1:21:A:VAL:HG23 | 7        | 0.12          |
| (3,972) | 1:21:A:VAL:H | 1:21:A:VAL:HG21 | 34       | 0.12          |
| (3,972) | 1:21:A:VAL:H | 1:21:A:VAL:HG22 | 34       | 0.12          |
| (3,972) | 1:21:A:VAL:H | 1:21:A:VAL:HG23 | 34       | 0.12          |
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 2        | 0.12          |
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 4        | 0.12          |
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 20       | 0.12          |
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 22       | 0.12          |
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 25       | 0.12          |
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 31       | 0.12          |
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 40       | 0.12          |
| (3,942) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 10       | 0.12          |
| (3,942) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 37       | 0.12          |
| (3,942) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 39       | 0.12          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 13       | 0.12          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 13       | 0.12          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 13       | 0.12          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 24       | 0.12          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 24       | 0.12          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 24       | 0.12          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 26       | 0.12          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 26       | 0.12          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 26       | 0.12          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 28       | 0.12          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 28       | 0.12          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 28       | 0.12          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 30       | 0.12          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 30       | 0.12          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 30       | 0.12          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 31       | 0.12          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 31       | 0.12          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 31       | 0.12          |
| (3,933) | 1:98:A:LYS:H | 1:19:A:ILE:HB   | 14       | 0.12          |
| (3,916) | 1:37:A:ASP:H | 1:37:A:ASP:HA   | 18       | 0.12          |
| (3,900) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 1        | 0.12          |
| (3,900) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 8        | 0.12          |
| (3,900) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 9        | 0.12          |
| (3,900) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 12       | 0.12          |
| (3,900) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 14       | 0.12          |
| (3,900) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 39       | 0.12          |
| (3,890) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 35       | 0.12          |
| (3,863) | 1:86:A:GLU:H | 1:85:A:LEU:HB3  | 22       | 0.12          |
| (3,863) | 1:86:A:GLU:H | 1:85:A:LEU:HB3  | 37       | 0.12          |
| (3,863) | 1:86:A:GLU:H | 1:85:A:LEU:HB3  | 38       | 0.12          |
| (3,863) | 1:86:A:GLU:H | 1:85:A:LEU:HB3  | 40       | 0.12          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 2        | 0.12          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 2        | 0.12          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 2        | 0.12          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 13       | 0.12          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 13       | 0.12          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 13       | 0.12          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 23       | 0.12          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 23       | 0.12          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 23       | 0.12          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 35       | 0.12          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 35       | 0.12          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 35       | 0.12          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 18       | 0.12          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 18       | 0.12          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 18       | 0.12          |
| (3,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB   | 1        | 0.12          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (3,810) | 1:25:A:GLN:H  | 1:71:A:VAL:HB   | 2        | 0.12          |
| (3,810) | 1:25:A:GLN:H  | 1:71:A:VAL:HB   | 3        | 0.12          |
| (3,810) | 1:25:A:GLN:H  | 1:71:A:VAL:HB   | 30       | 0.12          |
| (3,810) | 1:25:A:GLN:H  | 1:71:A:VAL:HB   | 32       | 0.12          |
| (3,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 10       | 0.12          |
| (3,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 16       | 0.12          |
| (3,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 23       | 0.12          |
| (3,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 24       | 0.12          |
| (3,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 25       | 0.12          |
| (3,726) | 1:49:A:LEU:H  | 1:48:A:GLU:HG3  | 40       | 0.12          |
| (3,709) | 1:16:A:ILE:H  | 1:31:A:CYS:HB2  | 21       | 0.12          |
| (3,709) | 1:16:A:ILE:H  | 1:31:A:CYS:HB2  | 34       | 0.12          |
| (3,683) | 1:23:A:GLU:H  | 1:22:A:SER:HB3  | 7        | 0.12          |
| (3,672) | 1:72:A:THR:H  | 1:73:A:PRO:HD2  | 17       | 0.12          |
| (3,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 1        | 0.12          |
| (3,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 7        | 0.12          |
| (3,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 10       | 0.12          |
| (3,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 19       | 0.12          |
| (3,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 28       | 0.12          |
| (3,661) | 1:7:A:ALA:H   | 1:6:A:THR:HA    | 5        | 0.12          |
| (3,661) | 1:7:A:ALA:H   | 1:6:A:THR:HA    | 10       | 0.12          |
| (3,661) | 1:7:A:ALA:H   | 1:6:A:THR:HA    | 31       | 0.12          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 12       | 0.12          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 13       | 0.12          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 18       | 0.12          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 20       | 0.12          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 30       | 0.12          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 35       | 0.12          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 36       | 0.12          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 37       | 0.12          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 14       | 0.12          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 16       | 0.12          |
| (3,609) | 1:43:A:TYR:H  | 1:42:A:TRP:HB2  | 12       | 0.12          |
| (3,609) | 1:43:A:TYR:H  | 1:42:A:TRP:HB2  | 19       | 0.12          |
| (3,609) | 1:43:A:TYR:H  | 1:42:A:TRP:HB2  | 29       | 0.12          |
| (3,589) | 1:93:A:SER:H  | 1:92:A:ARG:HG2  | 8        | 0.12          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 1        | 0.12          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 1        | 0.12          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 1        | 0.12          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 3        | 0.12          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 3        | 0.12          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 3        | 0.12          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 4        | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 4        | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 4        | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 7        | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 7        | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 7        | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 12       | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 12       | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 12       | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 13       | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 13       | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 13       | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 15       | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 15       | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 15       | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 16       | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 16       | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 16       | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 27       | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 27       | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 27       | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 32       | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 32       | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 32       | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 33       | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 33       | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 33       | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 37       | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 37       | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 37       | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 38       | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 38       | 0.12          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 38       | 0.12          |
| (3,560) | 1:47:A:THR:H | 1:47:A:THR:HA   | 11       | 0.12          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1  | 12       | 0.12          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2  | 12       | 0.12          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1  | 31       | 0.12          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2  | 31       | 0.12          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1  | 36       | 0.12          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2  | 36       | 0.12          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 11       | 0.12          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 11       | 0.12          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 11       | 0.12          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 16       | 0.12          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 16       | 0.12          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 16       | 0.12          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 18       | 0.12          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 18       | 0.12          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 18       | 0.12          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 20       | 0.12          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 20       | 0.12          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 20       | 0.12          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 23       | 0.12          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 23       | 0.12          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 23       | 0.12          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 27       | 0.12          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 27       | 0.12          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 27       | 0.12          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 29       | 0.12          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 29       | 0.12          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 29       | 0.12          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 33       | 0.12          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 33       | 0.12          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 33       | 0.12          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 35       | 0.12          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 35       | 0.12          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 35       | 0.12          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 40       | 0.12          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 40       | 0.12          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 40       | 0.12          |
| (3,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 2        | 0.12          |
| (3,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 7        | 0.12          |
| (3,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 25       | 0.12          |
| (3,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 27       | 0.12          |
| (3,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 30       | 0.12          |
| (3,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 32       | 0.12          |
| (3,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 36       | 0.12          |
| (3,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 40       | 0.12          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 1        | 0.12          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 4        | 0.12          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 7        | 0.12          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 8        | 0.12          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 12       | 0.12          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 13       | 0.12          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 14       | 0.12          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 16       | 0.12          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 20       | 0.12          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 21       | 0.12          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 22       | 0.12          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 23       | 0.12          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 24       | 0.12          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 25       | 0.12          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 26       | 0.12          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 27       | 0.12          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 30       | 0.12          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 31       | 0.12          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 32       | 0.12          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 33       | 0.12          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 35       | 0.12          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 36       | 0.12          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 37       | 0.12          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 38       | 0.12          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 40       | 0.12          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 2        | 0.12          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 8        | 0.12          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 5        | 0.12          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 9        | 0.12          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 14       | 0.12          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 15       | 0.12          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 34       | 0.12          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 19       | 0.12          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 21       | 0.12          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 28       | 0.12          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 29       | 0.12          |
| (3,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 20       | 0.12          |
| (3,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 26       | 0.12          |
| (3,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 27       | 0.12          |
| (3,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD21 | 7        | 0.12          |
| (3,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD22 | 7        | 0.12          |
| (3,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD23 | 7        | 0.12          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 5        | 0.12          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 14       | 0.12          |
| (3,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 17       | 0.12          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 6        | 0.12          |
| (3,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 15       | 0.12          |
| (3,393) | 1:77:A:GLY:H | 1:96:A:GLU:HA   | 19       | 0.12          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,393) | 1:77:A:GLY:H | 1:96:A:GLU:HA   | 37       | 0.12          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 2        | 0.12          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 2        | 0.12          |
| (3,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 2        | 0.12          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 8        | 0.12          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 8        | 0.12          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 8        | 0.12          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 22       | 0.12          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 22       | 0.12          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 22       | 0.12          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 26       | 0.12          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 26       | 0.12          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 26       | 0.12          |
| (3,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 6        | 0.12          |
| (3,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 7        | 0.12          |
| (3,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 10       | 0.12          |
| (3,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 15       | 0.12          |
| (3,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 17       | 0.12          |
| (3,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 22       | 0.12          |
| (3,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 23       | 0.12          |
| (3,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD1  | 7        | 0.12          |
| (3,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD2  | 7        | 0.12          |
| (3,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD1  | 10       | 0.12          |
| (3,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD2  | 10       | 0.12          |
| (3,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD1  | 33       | 0.12          |
| (3,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD2  | 33       | 0.12          |
| (3,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 3        | 0.12          |
| (3,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 4        | 0.12          |
| (3,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 21       | 0.12          |
| (3,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 24       | 0.12          |
| (3,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 39       | 0.12          |
| (3,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 40       | 0.12          |
| (3,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3  | 5        | 0.12          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 17       | 0.12          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 17       | 0.12          |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 17       | 0.12          |
| (3,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 2        | 0.12          |
| (3,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 6        | 0.12          |
| (3,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 7        | 0.12          |
| (3,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 9        | 0.12          |
| (3,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 11       | 0.12          |
| (3,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 19       | 0.12          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (3,239) | 1:13:A:THR:H  | 1:14:A:LYS:HA  | 20       | 0.12          |
| (3,239) | 1:13:A:THR:H  | 1:14:A:LYS:HA  | 21       | 0.12          |
| (3,239) | 1:13:A:THR:H  | 1:14:A:LYS:HA  | 23       | 0.12          |
| (3,239) | 1:13:A:THR:H  | 1:14:A:LYS:HA  | 25       | 0.12          |
| (3,239) | 1:13:A:THR:H  | 1:14:A:LYS:HA  | 27       | 0.12          |
| (3,239) | 1:13:A:THR:H  | 1:14:A:LYS:HA  | 33       | 0.12          |
| (3,239) | 1:13:A:THR:H  | 1:14:A:LYS:HA  | 38       | 0.12          |
| (3,239) | 1:13:A:THR:H  | 1:14:A:LYS:HA  | 39       | 0.12          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD1 | 2        | 0.12          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD2 | 2        | 0.12          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD1 | 5        | 0.12          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD2 | 5        | 0.12          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD1 | 10       | 0.12          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD2 | 10       | 0.12          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD1 | 23       | 0.12          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD2 | 23       | 0.12          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD1 | 29       | 0.12          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD2 | 29       | 0.12          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD1 | 30       | 0.12          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD2 | 30       | 0.12          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD1 | 36       | 0.12          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD2 | 36       | 0.12          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD1 | 37       | 0.12          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD2 | 37       | 0.12          |
| (3,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2 | 13       | 0.12          |
| (3,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2 | 17       | 0.12          |
| (3,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2 | 21       | 0.12          |
| (3,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2 | 24       | 0.12          |
| (3,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2 | 25       | 0.12          |
| (3,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2 | 30       | 0.12          |
| (3,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2 | 35       | 0.12          |
| (3,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2 | 40       | 0.12          |
| (3,165) | 1:10:A:ILE:H  | 1:9:A:PRO:HB2  | 16       | 0.12          |
| (3,165) | 1:10:A:ILE:H  | 1:9:A:PRO:HB2  | 20       | 0.12          |
| (3,141) | 1:101:A:LEU:H | 1:100:A:GLU:H  | 39       | 0.12          |
| (3,113) | 1:63:A:CYS:H  | 1:60:A:ASP:H   | 3        | 0.12          |
| (3,113) | 1:63:A:CYS:H  | 1:60:A:ASP:H   | 26       | 0.12          |
| (3,39)  | 1:88:A:ARG:H  | 1:88:A:ARG:HB3 | 25       | 0.12          |
| (3,39)  | 1:88:A:ARG:H  | 1:88:A:ARG:HB3 | 26       | 0.12          |
| (3,39)  | 1:88:A:ARG:H  | 1:88:A:ARG:HB3 | 27       | 0.12          |
| (3,39)  | 1:88:A:ARG:H  | 1:88:A:ARG:HB3 | 32       | 0.12          |
| (3,39)  | 1:88:A:ARG:H  | 1:88:A:ARG:HB3 | 33       | 0.12          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,39)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3  | 37       | 0.12          |
| (3,39)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3  | 39       | 0.12          |
| (3,25)   | 1:89:A:GLY:H   | 1:88:A:ARG:HB3  | 6        | 0.12          |
| (3,25)   | 1:89:A:GLY:H   | 1:88:A:ARG:HB3  | 9        | 0.12          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 9        | 0.12          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 9        | 0.12          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 24       | 0.12          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 24       | 0.12          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 25       | 0.12          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 25       | 0.12          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 27       | 0.12          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 27       | 0.12          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 29       | 0.12          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 29       | 0.12          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 34       | 0.12          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 34       | 0.12          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 36       | 0.12          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 36       | 0.12          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 38       | 0.12          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 38       | 0.12          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 4        | 0.12          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 4        | 0.12          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 4        | 0.12          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 4        | 0.12          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 4        | 0.12          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 4        | 0.12          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 22       | 0.12          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 22       | 0.12          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 22       | 0.12          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 22       | 0.12          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 22       | 0.12          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 22       | 0.12          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 26       | 0.12          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 26       | 0.12          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 26       | 0.12          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 26       | 0.12          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 26       | 0.12          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 26       | 0.12          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 31       | 0.12          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 31       | 0.12          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 31       | 0.12          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 31       | 0.12          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 31       | 0.12          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 31       | 0.12          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 36       | 0.12          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 36       | 0.12          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 36       | 0.12          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 36       | 0.12          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 36       | 0.12          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 36       | 0.12          |
| (1,3197) | 1:42:A:TRP:HZ2 | 1:30:A:GLU:HA   | 8        | 0.12          |
| (1,3197) | 1:42:A:TRP:HZ2 | 1:30:A:GLU:HA   | 20       | 0.12          |
| (1,3197) | 1:42:A:TRP:HZ2 | 1:30:A:GLU:HA   | 23       | 0.12          |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG21 | 5        | 0.12          |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG22 | 5        | 0.12          |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG23 | 5        | 0.12          |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG21 | 14       | 0.12          |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG22 | 14       | 0.12          |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG23 | 14       | 0.12          |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG21 | 27       | 0.12          |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG22 | 27       | 0.12          |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG23 | 27       | 0.12          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 11       | 0.12          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 11       | 0.12          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 11       | 0.12          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 11       | 0.12          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 17       | 0.12          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 17       | 0.12          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 17       | 0.12          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 17       | 0.12          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 20       | 0.12          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 20       | 0.12          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 20       | 0.12          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 20       | 0.12          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 23       | 0.12          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 23       | 0.12          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 23       | 0.12          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 23       | 0.12          |
| (1,3185) | 1:43:A:TYR:HD1 | 1:44:A:LYS:H    | 3        | 0.12          |
| (1,3185) | 1:43:A:TYR:HD2 | 1:44:A:LYS:H    | 3        | 0.12          |
| (1,3185) | 1:43:A:TYR:HD1 | 1:44:A:LYS:H    | 4        | 0.12          |
| (1,3185) | 1:43:A:TYR:HD2 | 1:44:A:LYS:H    | 4        | 0.12          |
| (1,3185) | 1:43:A:TYR:HD1 | 1:44:A:LYS:H    | 5        | 0.12          |
| (1,3185) | 1:43:A:TYR:HD2 | 1:44:A:LYS:H    | 5        | 0.12          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,3185) | 1:43:A:TYR:HD1 | 1:44:A:LYS:H   | 12       | 0.12          |
| (1,3185) | 1:43:A:TYR:HD2 | 1:44:A:LYS:H   | 12       | 0.12          |
| (1,3185) | 1:43:A:TYR:HD1 | 1:44:A:LYS:H   | 15       | 0.12          |
| (1,3185) | 1:43:A:TYR:HD2 | 1:44:A:LYS:H   | 15       | 0.12          |
| (1,3185) | 1:43:A:TYR:HD1 | 1:44:A:LYS:H   | 20       | 0.12          |
| (1,3185) | 1:43:A:TYR:HD2 | 1:44:A:LYS:H   | 20       | 0.12          |
| (1,3185) | 1:43:A:TYR:HD1 | 1:44:A:LYS:H   | 27       | 0.12          |
| (1,3185) | 1:43:A:TYR:HD2 | 1:44:A:LYS:H   | 27       | 0.12          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1 | 7        | 0.12          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2 | 7        | 0.12          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3 | 7        | 0.12          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1 | 10       | 0.12          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2 | 10       | 0.12          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3 | 10       | 0.12          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1 | 34       | 0.12          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2 | 34       | 0.12          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3 | 34       | 0.12          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1 | 38       | 0.12          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2 | 38       | 0.12          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3 | 38       | 0.12          |
| (1,3158) | 1:42:A:TRP:HD1 | 1:41:A:THR:HA  | 29       | 0.12          |
| (1,3158) | 1:42:A:TRP:HD1 | 1:41:A:THR:HA  | 40       | 0.12          |
| (1,3137) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3 | 9        | 0.12          |
| (1,3137) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3 | 9        | 0.12          |
| (1,3137) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3 | 22       | 0.12          |
| (1,3137) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3 | 22       | 0.12          |
| (1,3137) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3 | 24       | 0.12          |
| (1,3137) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3 | 24       | 0.12          |
| (1,3137) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3 | 32       | 0.12          |
| (1,3137) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3 | 32       | 0.12          |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 17       | 0.12          |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 17       | 0.12          |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2 | 20       | 0.12          |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2 | 20       | 0.12          |
| (1,3133) | 1:65:A:TYR:HE1 | 1:60:A:ASP:HB3 | 21       | 0.12          |
| (1,3133) | 1:65:A:TYR:HE2 | 1:60:A:ASP:HB3 | 21       | 0.12          |
| (1,3133) | 1:65:A:TYR:HE1 | 1:60:A:ASP:HB3 | 23       | 0.12          |
| (1,3133) | 1:65:A:TYR:HE2 | 1:60:A:ASP:HB3 | 23       | 0.12          |
| (1,3132) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB2 | 2        | 0.12          |
| (1,3132) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB2 | 2        | 0.12          |
| (1,3132) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB2 | 12       | 0.12          |
| (1,3132) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB2 | 12       | 0.12          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3132) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB2  | 13       | 0.12          |
| (1,3132) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB2  | 13       | 0.12          |
| (1,3132) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB2  | 21       | 0.12          |
| (1,3132) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB2  | 21       | 0.12          |
| (1,3131) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3  | 13       | 0.12          |
| (1,3131) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3  | 13       | 0.12          |
| (1,3131) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3  | 28       | 0.12          |
| (1,3131) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3  | 28       | 0.12          |
| (1,3131) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3  | 37       | 0.12          |
| (1,3131) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3  | 37       | 0.12          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 8        | 0.12          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 8        | 0.12          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 8        | 0.12          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 8        | 0.12          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 8        | 0.12          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 8        | 0.12          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 29       | 0.12          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 29       | 0.12          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 29       | 0.12          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 29       | 0.12          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 29       | 0.12          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 29       | 0.12          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 33       | 0.12          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 33       | 0.12          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 33       | 0.12          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 33       | 0.12          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 33       | 0.12          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 33       | 0.12          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 14       | 0.12          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 14       | 0.12          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 14       | 0.12          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 14       | 0.12          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 14       | 0.12          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 14       | 0.12          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 28       | 0.12          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 28       | 0.12          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 28       | 0.12          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 28       | 0.12          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 28       | 0.12          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 28       | 0.12          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 29       | 0.12          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 29       | 0.12          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 29       | 0.12          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 29       | 0.12          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 29       | 0.12          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 29       | 0.12          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 39       | 0.12          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 39       | 0.12          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 39       | 0.12          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 39       | 0.12          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 39       | 0.12          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 39       | 0.12          |
| (1,3104) | 1:79:A:TYR:HE1 | 1:66:A:MET:HE1  | 1        | 0.12          |
| (1,3104) | 1:79:A:TYR:HE1 | 1:66:A:MET:HE2  | 1        | 0.12          |
| (1,3104) | 1:79:A:TYR:HE1 | 1:66:A:MET:HE3  | 1        | 0.12          |
| (1,3104) | 1:79:A:TYR:HE2 | 1:66:A:MET:HE1  | 1        | 0.12          |
| (1,3104) | 1:79:A:TYR:HE2 | 1:66:A:MET:HE2  | 1        | 0.12          |
| (1,3104) | 1:79:A:TYR:HE2 | 1:66:A:MET:HE3  | 1        | 0.12          |
| (1,3104) | 1:79:A:TYR:HE1 | 1:66:A:MET:HE1  | 5        | 0.12          |
| (1,3104) | 1:79:A:TYR:HE1 | 1:66:A:MET:HE2  | 5        | 0.12          |
| (1,3104) | 1:79:A:TYR:HE1 | 1:66:A:MET:HE3  | 5        | 0.12          |
| (1,3104) | 1:79:A:TYR:HE2 | 1:66:A:MET:HE1  | 5        | 0.12          |
| (1,3104) | 1:79:A:TYR:HE2 | 1:66:A:MET:HE2  | 5        | 0.12          |
| (1,3104) | 1:79:A:TYR:HE2 | 1:66:A:MET:HE3  | 5        | 0.12          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 13       | 0.12          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 13       | 0.12          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 13       | 0.12          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 13       | 0.12          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 18       | 0.12          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 18       | 0.12          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 18       | 0.12          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 18       | 0.12          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 26       | 0.12          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 26       | 0.12          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 26       | 0.12          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 26       | 0.12          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 29       | 0.12          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 29       | 0.12          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 29       | 0.12          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 29       | 0.12          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 39       | 0.12          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 39       | 0.12          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 39       | 0.12          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 39       | 0.12          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 3        | 0.12          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 3        | 0.12          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 3        | 0.12          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 3        | 0.12          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 3        | 0.12          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 3        | 0.12          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 5        | 0.12          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 5        | 0.12          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 5        | 0.12          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 5        | 0.12          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 5        | 0.12          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 5        | 0.12          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 15       | 0.12          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 15       | 0.12          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 15       | 0.12          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 15       | 0.12          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 15       | 0.12          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 15       | 0.12          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 23       | 0.12          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 23       | 0.12          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 23       | 0.12          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 23       | 0.12          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 23       | 0.12          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 23       | 0.12          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 26       | 0.12          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 26       | 0.12          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 26       | 0.12          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 26       | 0.12          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 26       | 0.12          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 26       | 0.12          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 14       | 0.12          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 14       | 0.12          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 14       | 0.12          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 20       | 0.12          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 20       | 0.12          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 20       | 0.12          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 23       | 0.12          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 23       | 0.12          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 23       | 0.12          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 25       | 0.12          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 25       | 0.12          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 25       | 0.12          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 30       | 0.12          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 30       | 0.12          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 30       | 0.12          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 35       | 0.12          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 35       | 0.12          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 35       | 0.12          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 36       | 0.12          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 36       | 0.12          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 36       | 0.12          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 39       | 0.12          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 39       | 0.12          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 39       | 0.12          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 9        | 0.12          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 9        | 0.12          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 30       | 0.12          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 30       | 0.12          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 33       | 0.12          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 33       | 0.12          |
| (1,3040) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG21 | 24       | 0.12          |
| (1,3040) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG22 | 24       | 0.12          |
| (1,3040) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG23 | 24       | 0.12          |
| (1,3040) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG21 | 28       | 0.12          |
| (1,3040) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG22 | 28       | 0.12          |
| (1,3040) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG23 | 28       | 0.12          |
| (1,3040) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG21 | 39       | 0.12          |
| (1,3040) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG22 | 39       | 0.12          |
| (1,3040) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG23 | 39       | 0.12          |
| (1,3033) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE1  | 33       | 0.12          |
| (1,3033) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE2  | 33       | 0.12          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 4        | 0.12          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 4        | 0.12          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 6        | 0.12          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 6        | 0.12          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 15       | 0.12          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 15       | 0.12          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 16       | 0.12          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 16       | 0.12          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 31       | 0.12          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 31       | 0.12          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 39       | 0.12          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 39       | 0.12          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 11       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG22 | 11       | 0.12          |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG23 | 11       | 0.12          |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG21 | 12       | 0.12          |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG22 | 12       | 0.12          |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG23 | 12       | 0.12          |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG21 | 35       | 0.12          |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG22 | 35       | 0.12          |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG23 | 35       | 0.12          |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG21 | 38       | 0.12          |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG22 | 38       | 0.12          |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG23 | 38       | 0.12          |
| (1,3011) | 1:30:A:GLU:HB2  | 1:14:A:LYS:HE2  | 2        | 0.12          |
| (1,3011) | 1:30:A:GLU:HB2  | 1:14:A:LYS:HE2  | 3        | 0.12          |
| (1,3011) | 1:30:A:GLU:HB2  | 1:14:A:LYS:HE2  | 19       | 0.12          |
| (1,3011) | 1:30:A:GLU:HB2  | 1:14:A:LYS:HE2  | 40       | 0.12          |
| (1,3009) | 1:102:A:ARG:HD3 | 1:102:A:ARG:HB2 | 25       | 0.12          |
| (1,2996) | 1:15:A:ARG:HG2  | 1:93:A:SER:HB3  | 21       | 0.12          |
| (1,2996) | 1:15:A:ARG:HG2  | 1:93:A:SER:HB3  | 22       | 0.12          |
| (1,2996) | 1:15:A:ARG:HG2  | 1:93:A:SER:HB3  | 33       | 0.12          |
| (1,2974) | 1:65:A:TYR:HA   | 1:42:A:TRP:HZ2  | 4        | 0.12          |
| (1,2974) | 1:65:A:TYR:HA   | 1:42:A:TRP:HZ2  | 10       | 0.12          |
| (1,2974) | 1:65:A:TYR:HA   | 1:42:A:TRP:HZ2  | 26       | 0.12          |
| (1,2974) | 1:65:A:TYR:HA   | 1:42:A:TRP:HZ2  | 39       | 0.12          |
| (1,2974) | 1:65:A:TYR:HA   | 1:42:A:TRP:HZ2  | 40       | 0.12          |
| (1,2967) | 1:44:A:LYS:HE3  | 1:44:A:LYS:HD2  | 35       | 0.12          |
| (1,2953) | 1:98:A:LYS:HB3  | 1:98:A:LYS:HG2  | 1        | 0.12          |
| (1,2953) | 1:98:A:LYS:HB3  | 1:98:A:LYS:HG2  | 9        | 0.12          |
| (1,2953) | 1:98:A:LYS:HB3  | 1:98:A:LYS:HG2  | 11       | 0.12          |
| (1,2953) | 1:98:A:LYS:HB3  | 1:98:A:LYS:HG2  | 16       | 0.12          |
| (1,2953) | 1:98:A:LYS:HB3  | 1:98:A:LYS:HG2  | 17       | 0.12          |
| (1,2953) | 1:98:A:LYS:HB3  | 1:98:A:LYS:HG2  | 22       | 0.12          |
| (1,2953) | 1:98:A:LYS:HB3  | 1:98:A:LYS:HG2  | 25       | 0.12          |
| (1,2953) | 1:98:A:LYS:HB3  | 1:98:A:LYS:HG2  | 31       | 0.12          |
| (1,2953) | 1:98:A:LYS:HB3  | 1:98:A:LYS:HG2  | 37       | 0.12          |
| (1,2953) | 1:98:A:LYS:HB3  | 1:98:A:LYS:HG2  | 38       | 0.12          |
| (1,2949) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 2        | 0.12          |
| (1,2949) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 11       | 0.12          |
| (1,2949) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 18       | 0.12          |
| (1,2949) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 19       | 0.12          |
| (1,2949) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 20       | 0.12          |
| (1,2949) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 22       | 0.12          |
| (1,2949) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 24       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2949) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 32       | 0.12          |
| (1,2949) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 35       | 0.12          |
| (1,2949) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 38       | 0.12          |
| (1,2942) | 1:90:A:GLU:HA   | 1:84:A:ARG:HA   | 15       | 0.12          |
| (1,2937) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD1  | 9        | 0.12          |
| (1,2937) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD2  | 9        | 0.12          |
| (1,2937) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD1  | 22       | 0.12          |
| (1,2937) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD2  | 22       | 0.12          |
| (1,2937) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD1  | 24       | 0.12          |
| (1,2937) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD2  | 24       | 0.12          |
| (1,2937) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD1  | 32       | 0.12          |
| (1,2937) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD2  | 32       | 0.12          |
| (1,2931) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 9        | 0.12          |
| (1,2931) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 13       | 0.12          |
| (1,2931) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 19       | 0.12          |
| (1,2931) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 20       | 0.12          |
| (1,2931) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 27       | 0.12          |
| (1,2931) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 33       | 0.12          |
| (1,2903) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HD2  | 16       | 0.12          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 4        | 0.12          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 5        | 0.12          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 6        | 0.12          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 11       | 0.12          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 12       | 0.12          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 13       | 0.12          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 16       | 0.12          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 17       | 0.12          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 21       | 0.12          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 24       | 0.12          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 27       | 0.12          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 29       | 0.12          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 33       | 0.12          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 35       | 0.12          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 38       | 0.12          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 39       | 0.12          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 40       | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 1        | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 2        | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 3        | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 4        | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 6        | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 8        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 10       | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 11       | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 12       | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 13       | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 14       | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 15       | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 16       | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 17       | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 18       | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 21       | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 22       | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 23       | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 24       | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 25       | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 26       | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 27       | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 28       | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 30       | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 31       | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 32       | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 33       | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 34       | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 35       | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 36       | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 37       | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 38       | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 39       | 0.12          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 40       | 0.12          |
| (1,2859) | 1:92:A:ARG:HB3  | 1:92:A:ARG:H    | 27       | 0.12          |
| (1,2841) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA   | 26       | 0.12          |
| (1,2841) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA   | 34       | 0.12          |
| (1,2822) | 1:58:A:ARG:HD3  | 1:58:A:ARG:HG2  | 21       | 0.12          |
| (1,2802) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HB2  | 6        | 0.12          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 12       | 0.12          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 13       | 0.12          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 18       | 0.12          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 20       | 0.12          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 30       | 0.12          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 35       | 0.12          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 36       | 0.12          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 37       | 0.12          |
| (1,2754) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 2        | 0.12          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,2754) | 1:90:A:GLU:HB3 | 1:91:A:ALA:H   | 15       | 0.12          |
| (1,2754) | 1:90:A:GLU:HB3 | 1:91:A:ALA:H   | 16       | 0.12          |
| (1,2754) | 1:90:A:GLU:HB3 | 1:91:A:ALA:H   | 17       | 0.12          |
| (1,2745) | 1:86:A:GLU:HG2 | 1:86:A:GLU:H   | 29       | 0.12          |
| (1,2745) | 1:86:A:GLU:HG3 | 1:86:A:GLU:H   | 29       | 0.12          |
| (1,2723) | 1:76:A:GLU:HB2 | 1:77:A:GLY:H   | 5        | 0.12          |
| (1,2723) | 1:76:A:GLU:HB2 | 1:77:A:GLY:H   | 14       | 0.12          |
| (1,2723) | 1:76:A:GLU:HB2 | 1:77:A:GLY:H   | 17       | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 1        | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 2        | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 3        | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 4        | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 5        | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 6        | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 10       | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 12       | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 13       | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 15       | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 16       | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 17       | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 18       | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 19       | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 21       | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 22       | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 23       | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 24       | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 25       | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 26       | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 27       | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 28       | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 30       | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 31       | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 32       | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 33       | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 34       | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 36       | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 37       | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 38       | 0.12          |
| (1,2713) | 1:48:A:GLU:HA  | 1:48:A:GLU:HG3 | 40       | 0.12          |
| (1,2699) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA  | 1        | 0.12          |
| (1,2699) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA  | 10       | 0.12          |
| (1,2699) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA  | 11       | 0.12          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,2699) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA  | 15       | 0.12          |
| (1,2699) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA  | 16       | 0.12          |
| (1,2699) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA  | 21       | 0.12          |
| (1,2699) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA  | 22       | 0.12          |
| (1,2699) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA  | 25       | 0.12          |
| (1,2699) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA  | 26       | 0.12          |
| (1,2699) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA  | 27       | 0.12          |
| (1,2699) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA  | 30       | 0.12          |
| (1,2699) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA  | 32       | 0.12          |
| (1,2699) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA  | 35       | 0.12          |
| (1,2699) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA  | 40       | 0.12          |
| (1,2686) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2  | 3        | 0.12          |
| (1,2686) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2  | 12       | 0.12          |
| (1,2686) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2  | 15       | 0.12          |
| (1,2686) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2  | 25       | 0.12          |
| (1,2686) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2  | 29       | 0.12          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 1        | 0.12          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 2        | 0.12          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 3        | 0.12          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 6        | 0.12          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 7        | 0.12          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 11       | 0.12          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 12       | 0.12          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 13       | 0.12          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 14       | 0.12          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 17       | 0.12          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 18       | 0.12          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 19       | 0.12          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 20       | 0.12          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 22       | 0.12          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 25       | 0.12          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 26       | 0.12          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 27       | 0.12          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 28       | 0.12          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 29       | 0.12          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 30       | 0.12          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 31       | 0.12          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 32       | 0.12          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 33       | 0.12          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 34       | 0.12          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 36       | 0.12          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2 | 37       | 0.12          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 38       | 0.12          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 39       | 0.12          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 40       | 0.12          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 3        | 0.12          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 3        | 0.12          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 3        | 0.12          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 8        | 0.12          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 8        | 0.12          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 8        | 0.12          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 28       | 0.12          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 28       | 0.12          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 28       | 0.12          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 39       | 0.12          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 39       | 0.12          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 39       | 0.12          |
| (1,2649) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 6        | 0.12          |
| (1,2649) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 7        | 0.12          |
| (1,2649) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 10       | 0.12          |
| (1,2649) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 15       | 0.12          |
| (1,2649) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 17       | 0.12          |
| (1,2649) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 22       | 0.12          |
| (1,2649) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 23       | 0.12          |
| (1,2646) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3   | 21       | 0.12          |
| (1,2646) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3   | 22       | 0.12          |
| (1,2646) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3   | 24       | 0.12          |
| (1,2646) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3   | 32       | 0.12          |
| (1,2646) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3   | 35       | 0.12          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3   | 22       | 0.12          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3   | 32       | 0.12          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3   | 35       | 0.12          |
| (1,2609) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 6        | 0.12          |
| (1,2609) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 13       | 0.12          |
| (1,2608) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 6        | 0.12          |
| (1,2608) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 13       | 0.12          |
| (1,2550) | 1:92:A:ARG:HA  | 1:83:A:ALA:H    | 2        | 0.12          |
| (1,2550) | 1:92:A:ARG:HA  | 1:83:A:ALA:H    | 10       | 0.12          |
| (1,2550) | 1:92:A:ARG:HA  | 1:83:A:ALA:H    | 11       | 0.12          |
| (1,2550) | 1:92:A:ARG:HA  | 1:83:A:ALA:H    | 13       | 0.12          |
| (1,2550) | 1:92:A:ARG:HA  | 1:83:A:ALA:H    | 22       | 0.12          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA   | 11       | 0.12          |
| (1,2539) | 1:73:A:PRO:HG2 | 1:73:A:PRO:HA   | 18       | 0.12          |
| (1,2537) | 1:73:A:PRO:HG3 | 1:73:A:PRO:HA   | 22       | 0.12          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,2537) | 1:73:A:PRO:HG3 | 1:73:A:PRO:HA   | 33       | 0.12          |
| (1,2537) | 1:73:A:PRO:HG3 | 1:73:A:PRO:HA   | 39       | 0.12          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2   | 26       | 0.12          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2   | 28       | 0.12          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2   | 33       | 0.12          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA    | 21       | 0.12          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA    | 22       | 0.12          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA    | 23       | 0.12          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA    | 24       | 0.12          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA    | 25       | 0.12          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA    | 27       | 0.12          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA    | 30       | 0.12          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA    | 32       | 0.12          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA    | 34       | 0.12          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA    | 38       | 0.12          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA    | 40       | 0.12          |
| (1,2479) | 1:9:A:PRO:HD2  | 1:8:A:GLU:HA    | 1        | 0.12          |
| (1,2479) | 1:9:A:PRO:HD2  | 1:8:A:GLU:HA    | 20       | 0.12          |
| (1,2479) | 1:9:A:PRO:HD2  | 1:8:A:GLU:HA    | 33       | 0.12          |
| (1,2460) | 1:4:A:PRO:HD3  | 1:3:A:ASP:HA    | 8        | 0.12          |
| (1,2460) | 1:4:A:PRO:HD3  | 1:3:A:ASP:HA    | 9        | 0.12          |
| (1,2460) | 1:4:A:PRO:HD3  | 1:3:A:ASP:HA    | 25       | 0.12          |
| (1,2431) | 1:82:A:ILE:HB  | 1:41:A:THR:H    | 10       | 0.12          |
| (1,2431) | 1:82:A:ILE:HB  | 1:41:A:THR:H    | 15       | 0.12          |
| (1,2424) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD11 | 38       | 0.12          |
| (1,2424) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD12 | 38       | 0.12          |
| (1,2424) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD13 | 38       | 0.12          |
| (1,2416) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 5        | 0.12          |
| (1,2416) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 9        | 0.12          |
| (1,2416) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 11       | 0.12          |
| (1,2416) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 17       | 0.12          |
| (1,2416) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 27       | 0.12          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2  | 15       | 0.12          |
| (1,2409) | 1:10:A:ILE:HA  | 1:11:A:GLN:HG2  | 19       | 0.12          |
| (1,2403) | 1:66:A:MET:HE1 | 1:42:A:TRP:H    | 6        | 0.12          |
| (1,2403) | 1:66:A:MET:HE2 | 1:42:A:TRP:H    | 6        | 0.12          |
| (1,2403) | 1:66:A:MET:HE3 | 1:42:A:TRP:H    | 6        | 0.12          |
| (1,2403) | 1:66:A:MET:HE1 | 1:42:A:TRP:H    | 40       | 0.12          |
| (1,2403) | 1:66:A:MET:HE2 | 1:42:A:TRP:H    | 40       | 0.12          |
| (1,2403) | 1:66:A:MET:HE3 | 1:42:A:TRP:H    | 40       | 0.12          |
| (1,2402) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ   | 4        | 0.12          |
| (1,2402) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ   | 4        | 0.12          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,2402) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ   | 4        | 0.12          |
| (1,2402) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ   | 24       | 0.12          |
| (1,2402) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ   | 24       | 0.12          |
| (1,2402) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ   | 24       | 0.12          |
| (1,2339) | 1:26:A:SER:HB3 | 1:27:A:ALA:H    | 11       | 0.12          |
| (1,2339) | 1:26:A:SER:HB3 | 1:27:A:ALA:H    | 30       | 0.12          |
| (1,2331) | 1:26:A:SER:HA  | 1:68:A:ILE:HG21 | 4        | 0.12          |
| (1,2331) | 1:26:A:SER:HA  | 1:68:A:ILE:HG22 | 4        | 0.12          |
| (1,2331) | 1:26:A:SER:HA  | 1:68:A:ILE:HG23 | 4        | 0.12          |
| (1,2331) | 1:26:A:SER:HA  | 1:68:A:ILE:HG21 | 22       | 0.12          |
| (1,2331) | 1:26:A:SER:HA  | 1:68:A:ILE:HG22 | 22       | 0.12          |
| (1,2331) | 1:26:A:SER:HA  | 1:68:A:ILE:HG23 | 22       | 0.12          |
| (1,2331) | 1:26:A:SER:HA  | 1:68:A:ILE:HG21 | 25       | 0.12          |
| (1,2331) | 1:26:A:SER:HA  | 1:68:A:ILE:HG22 | 25       | 0.12          |
| (1,2331) | 1:26:A:SER:HA  | 1:68:A:ILE:HG23 | 25       | 0.12          |
| (1,2287) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H    | 4        | 0.12          |
| (1,2287) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H    | 8        | 0.12          |
| (1,2287) | 1:96:A:GLU:HG2 | 1:96:A:GLU:H    | 29       | 0.12          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG21 | 3        | 0.12          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG22 | 3        | 0.12          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG23 | 3        | 0.12          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG21 | 9        | 0.12          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG22 | 9        | 0.12          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG23 | 9        | 0.12          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG21 | 10       | 0.12          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG22 | 10       | 0.12          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG23 | 10       | 0.12          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG21 | 12       | 0.12          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG22 | 12       | 0.12          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG23 | 12       | 0.12          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG21 | 16       | 0.12          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG22 | 16       | 0.12          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG23 | 16       | 0.12          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG21 | 27       | 0.12          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG22 | 27       | 0.12          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG23 | 27       | 0.12          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG21 | 35       | 0.12          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG22 | 35       | 0.12          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG23 | 35       | 0.12          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG21 | 36       | 0.12          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG22 | 36       | 0.12          |
| (1,2265) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG23 | 36       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG21 | 37       | 0.12          |
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG22 | 37       | 0.12          |
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG23 | 37       | 0.12          |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD11 | 28       | 0.12          |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD12 | 28       | 0.12          |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD13 | 28       | 0.12          |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD11 | 38       | 0.12          |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD12 | 38       | 0.12          |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD13 | 38       | 0.12          |
| (1,2150) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 16       | 0.12          |
| (1,2150) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 33       | 0.12          |
| (1,2145) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 6        | 0.12          |
| (1,2145) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 10       | 0.12          |
| (1,2145) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 22       | 0.12          |
| (1,2145) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 29       | 0.12          |
| (1,2145) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 31       | 0.12          |
| (1,2145) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 32       | 0.12          |
| (1,2145) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 36       | 0.12          |
| (1,2099) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HA   | 7        | 0.12          |
| (1,2099) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HA   | 7        | 0.12          |
| (1,2099) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HA   | 7        | 0.12          |
| (1,2099) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HA   | 30       | 0.12          |
| (1,2099) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HA   | 30       | 0.12          |
| (1,2099) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HA   | 30       | 0.12          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 6        | 0.12          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 6        | 0.12          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 6        | 0.12          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 15       | 0.12          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 15       | 0.12          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 15       | 0.12          |
| (1,2093) | 1:88:A:ARG:HD3  | 1:7:A:ALA:HA    | 40       | 0.12          |
| (1,2087) | 1:85:A:LEU:HD11 | 1:39:A:ILE:H    | 2        | 0.12          |
| (1,2087) | 1:85:A:LEU:HD12 | 1:39:A:ILE:H    | 2        | 0.12          |
| (1,2087) | 1:85:A:LEU:HD13 | 1:39:A:ILE:H    | 2        | 0.12          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1  | 5        | 0.12          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2  | 5        | 0.12          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1  | 5        | 0.12          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2  | 5        | 0.12          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1  | 5        | 0.12          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2  | 5        | 0.12          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1  | 8        | 0.12          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2  | 8        | 0.12          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1 | 8        | 0.12          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2 | 8        | 0.12          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1 | 8        | 0.12          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2 | 8        | 0.12          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1 | 14       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2 | 14       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1 | 14       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2 | 14       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1 | 14       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2 | 14       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1 | 21       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2 | 21       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1 | 21       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2 | 21       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1 | 21       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2 | 21       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1 | 22       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2 | 22       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1 | 22       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2 | 22       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1 | 22       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2 | 22       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1 | 25       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2 | 25       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1 | 25       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2 | 25       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1 | 25       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2 | 25       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1 | 31       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2 | 31       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1 | 31       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2 | 31       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1 | 31       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2 | 31       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1 | 36       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2 | 36       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1 | 36       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2 | 36       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1 | 36       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2 | 36       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1 | 37       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2 | 37       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1  | 37       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2  | 37       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1  | 37       | 0.12          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2  | 37       | 0.12          |
| (1,2076) | 1:97:A:LEU:HD11 | 1:21:A:VAL:HB   | 9        | 0.12          |
| (1,2076) | 1:97:A:LEU:HD12 | 1:21:A:VAL:HB   | 9        | 0.12          |
| (1,2076) | 1:97:A:LEU:HD13 | 1:21:A:VAL:HB   | 9        | 0.12          |
| (1,2068) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 16       | 0.12          |
| (1,2068) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 16       | 0.12          |
| (1,2068) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 16       | 0.12          |
| (1,2068) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 40       | 0.12          |
| (1,2068) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 40       | 0.12          |
| (1,2068) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 40       | 0.12          |
| (1,2054) | 1:78:A:VAL:HG11 | 1:96:A:GLU:HG2  | 38       | 0.12          |
| (1,2054) | 1:78:A:VAL:HG12 | 1:96:A:GLU:HG2  | 38       | 0.12          |
| (1,2054) | 1:78:A:VAL:HG13 | 1:96:A:GLU:HG2  | 38       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD21 | 19       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD22 | 19       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD23 | 19       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD21 | 19       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD22 | 19       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD23 | 19       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD21 | 19       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD22 | 19       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD23 | 19       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD21 | 25       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD22 | 25       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD23 | 25       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD21 | 25       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD22 | 25       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD23 | 25       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD21 | 25       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD22 | 25       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD23 | 25       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD21 | 30       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD22 | 30       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD23 | 30       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD21 | 30       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD22 | 30       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD23 | 30       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD21 | 30       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD22 | 30       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD23 | 30       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD21 | 32       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD22 | 32       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD23 | 32       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD21 | 32       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD22 | 32       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD23 | 32       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD21 | 32       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD22 | 32       | 0.12          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD23 | 32       | 0.12          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1  | 6        | 0.12          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2  | 6        | 0.12          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1  | 6        | 0.12          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2  | 6        | 0.12          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1  | 6        | 0.12          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2  | 6        | 0.12          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1  | 12       | 0.12          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2  | 12       | 0.12          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1  | 12       | 0.12          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2  | 12       | 0.12          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1  | 12       | 0.12          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2  | 12       | 0.12          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1  | 24       | 0.12          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2  | 24       | 0.12          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1  | 24       | 0.12          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2  | 24       | 0.12          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1  | 24       | 0.12          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2  | 24       | 0.12          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1  | 40       | 0.12          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2  | 40       | 0.12          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1  | 40       | 0.12          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2  | 40       | 0.12          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1  | 40       | 0.12          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2  | 40       | 0.12          |
| (1,2022) | 1:50:A:THR:HG21 | 1:57:A:PHE:HZ   | 34       | 0.12          |
| (1,2022) | 1:50:A:THR:HG22 | 1:57:A:PHE:HZ   | 34       | 0.12          |
| (1,2022) | 1:50:A:THR:HG23 | 1:57:A:PHE:HZ   | 34       | 0.12          |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3  | 3        | 0.12          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3  | 3        | 0.12          |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3  | 3        | 0.12          |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3  | 5        | 0.12          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3  | 5        | 0.12          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 5        | 0.12          |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 7        | 0.12          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 7        | 0.12          |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 7        | 0.12          |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 20       | 0.12          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 20       | 0.12          |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 20       | 0.12          |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 21       | 0.12          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 21       | 0.12          |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 21       | 0.12          |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 23       | 0.12          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 23       | 0.12          |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 23       | 0.12          |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 25       | 0.12          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 25       | 0.12          |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 25       | 0.12          |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 32       | 0.12          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 32       | 0.12          |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 32       | 0.12          |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 34       | 0.12          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 34       | 0.12          |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 34       | 0.12          |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 36       | 0.12          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 36       | 0.12          |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 36       | 0.12          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 9        | 0.12          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 9        | 0.12          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 9        | 0.12          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 9        | 0.12          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 9        | 0.12          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 9        | 0.12          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 27       | 0.12          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 27       | 0.12          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 27       | 0.12          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 27       | 0.12          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 27       | 0.12          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 27       | 0.12          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 31       | 0.12          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 31       | 0.12          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 31       | 0.12          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 31       | 0.12          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 31       | 0.12          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 31       | 0.12          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 37       | 0.12          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 37       | 0.12          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 37       | 0.12          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 37       | 0.12          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 37       | 0.12          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 37       | 0.12          |
| (1,2014) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD1 | 15       | 0.12          |
| (1,2014) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD2 | 15       | 0.12          |
| (1,2014) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD1 | 33       | 0.12          |
| (1,2014) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD2 | 33       | 0.12          |
| (1,2012) | 1:40:A:VAL:HG11 | 1:64:A:HIS:HD2 | 27       | 0.12          |
| (1,2012) | 1:40:A:VAL:HG12 | 1:64:A:HIS:HD2 | 27       | 0.12          |
| (1,2012) | 1:40:A:VAL:HG13 | 1:64:A:HIS:HD2 | 27       | 0.12          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1 | 6        | 0.12          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2 | 6        | 0.12          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3 | 6        | 0.12          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1 | 6        | 0.12          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2 | 6        | 0.12          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3 | 6        | 0.12          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1 | 6        | 0.12          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2 | 6        | 0.12          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3 | 6        | 0.12          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1 | 23       | 0.12          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2 | 23       | 0.12          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3 | 23       | 0.12          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1 | 23       | 0.12          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2 | 23       | 0.12          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3 | 23       | 0.12          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1 | 23       | 0.12          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2 | 23       | 0.12          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3 | 23       | 0.12          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 3        | 0.12          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 4        | 0.12          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 21       | 0.12          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 24       | 0.12          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 39       | 0.12          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 40       | 0.12          |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2 | 12       | 0.12          |
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2 | 12       | 0.12          |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2 | 12       | 0.12          |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2 | 13       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 13       | 0.12          |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 13       | 0.12          |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 40       | 0.12          |
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 40       | 0.12          |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 40       | 0.12          |
| (1,1994) | 1:21:A:VAL:HG11 | 1:25:A:GLN:HG3  | 37       | 0.12          |
| (1,1994) | 1:21:A:VAL:HG12 | 1:25:A:GLN:HG3  | 37       | 0.12          |
| (1,1994) | 1:21:A:VAL:HG13 | 1:25:A:GLN:HG3  | 37       | 0.12          |
| (1,1990) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 1        | 0.12          |
| (1,1990) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 1        | 0.12          |
| (1,1990) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 1        | 0.12          |
| (1,1990) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 16       | 0.12          |
| (1,1990) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 16       | 0.12          |
| (1,1990) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 16       | 0.12          |
| (1,1990) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 19       | 0.12          |
| (1,1990) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 19       | 0.12          |
| (1,1990) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 19       | 0.12          |
| (1,1990) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 35       | 0.12          |
| (1,1990) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 35       | 0.12          |
| (1,1990) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 35       | 0.12          |
| (1,1990) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 38       | 0.12          |
| (1,1990) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 38       | 0.12          |
| (1,1990) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 38       | 0.12          |
| (1,1966) | 1:36:A:ASP:HB3  | 1:62:A:ARG:HA   | 31       | 0.12          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 20       | 0.12          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 36       | 0.12          |
| (1,1952) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB1  | 15       | 0.12          |
| (1,1952) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB2  | 15       | 0.12          |
| (1,1952) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB3  | 15       | 0.12          |
| (1,1952) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB1  | 15       | 0.12          |
| (1,1952) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB2  | 15       | 0.12          |
| (1,1952) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB3  | 15       | 0.12          |
| (1,1952) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB1  | 15       | 0.12          |
| (1,1952) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB2  | 15       | 0.12          |
| (1,1952) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB3  | 15       | 0.12          |
| (1,1952) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB1  | 34       | 0.12          |
| (1,1952) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB2  | 34       | 0.12          |
| (1,1952) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB3  | 34       | 0.12          |
| (1,1952) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB1  | 34       | 0.12          |
| (1,1952) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB2  | 34       | 0.12          |
| (1,1952) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB3  | 34       | 0.12          |
| (1,1952) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB1  | 34       | 0.12          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1952) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB2 | 34       | 0.12          |
| (1,1952) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB3 | 34       | 0.12          |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 8        | 0.12          |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 8        | 0.12          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 8        | 0.12          |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 11       | 0.12          |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 11       | 0.12          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 11       | 0.12          |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 12       | 0.12          |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 12       | 0.12          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 12       | 0.12          |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 24       | 0.12          |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 24       | 0.12          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 24       | 0.12          |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 27       | 0.12          |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 27       | 0.12          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 27       | 0.12          |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 30       | 0.12          |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 30       | 0.12          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 30       | 0.12          |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 34       | 0.12          |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 34       | 0.12          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 34       | 0.12          |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 39       | 0.12          |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 39       | 0.12          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 39       | 0.12          |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 12       | 0.12          |
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 12       | 0.12          |
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 12       | 0.12          |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 18       | 0.12          |
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 18       | 0.12          |
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 18       | 0.12          |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 21       | 0.12          |
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 21       | 0.12          |
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 21       | 0.12          |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 24       | 0.12          |
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 24       | 0.12          |
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 24       | 0.12          |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 26       | 0.12          |
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 26       | 0.12          |
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 26       | 0.12          |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 27       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA   | 27       | 0.12          |
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA   | 27       | 0.12          |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA   | 37       | 0.12          |
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA   | 37       | 0.12          |
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA   | 37       | 0.12          |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA   | 38       | 0.12          |
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA   | 38       | 0.12          |
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA   | 38       | 0.12          |
| (1,1896) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3  | 4        | 0.12          |
| (1,1896) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3  | 4        | 0.12          |
| (1,1896) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3  | 4        | 0.12          |
| (1,1896) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3  | 8        | 0.12          |
| (1,1896) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3  | 8        | 0.12          |
| (1,1896) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3  | 8        | 0.12          |
| (1,1896) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3  | 11       | 0.12          |
| (1,1896) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3  | 11       | 0.12          |
| (1,1896) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3  | 11       | 0.12          |
| (1,1896) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3  | 38       | 0.12          |
| (1,1896) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3  | 38       | 0.12          |
| (1,1896) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3  | 38       | 0.12          |
| (1,1882) | 1:23:A:GLU:HG3  | 1:72:A:THR:HA   | 29       | 0.12          |
| (1,1861) | 1:7:A:ALA:HB1   | 1:88:A:ARG:HA   | 3        | 0.12          |
| (1,1861) | 1:7:A:ALA:HB2   | 1:88:A:ARG:HA   | 3        | 0.12          |
| (1,1861) | 1:7:A:ALA:HB3   | 1:88:A:ARG:HA   | 3        | 0.12          |
| (1,1853) | 1:27:A:ALA:HB1  | 1:28:A:THR:H    | 9        | 0.12          |
| (1,1853) | 1:27:A:ALA:HB2  | 1:28:A:THR:H    | 9        | 0.12          |
| (1,1853) | 1:27:A:ALA:HB3  | 1:28:A:THR:H    | 9        | 0.12          |
| (1,1803) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HB3  | 1        | 0.12          |
| (1,1803) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HB3  | 9        | 0.12          |
| (1,1803) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HB3  | 11       | 0.12          |
| (1,1803) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HB3  | 16       | 0.12          |
| (1,1803) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HB3  | 17       | 0.12          |
| (1,1803) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HB3  | 22       | 0.12          |
| (1,1803) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HB3  | 25       | 0.12          |
| (1,1803) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HB3  | 31       | 0.12          |
| (1,1803) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HB3  | 37       | 0.12          |
| (1,1803) | 1:98:A:LYS:HG2  | 1:98:A:LYS:HB3  | 38       | 0.12          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG11 | 3        | 0.12          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG12 | 3        | 0.12          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG13 | 3        | 0.12          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG11 | 3        | 0.12          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG12 | 3        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 3        | 0.12          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 3        | 0.12          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 3        | 0.12          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 3        | 0.12          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG11 | 8        | 0.12          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG12 | 8        | 0.12          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG13 | 8        | 0.12          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG11 | 8        | 0.12          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG12 | 8        | 0.12          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 8        | 0.12          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 8        | 0.12          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 8        | 0.12          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 8        | 0.12          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG11 | 12       | 0.12          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG12 | 12       | 0.12          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG13 | 12       | 0.12          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG11 | 12       | 0.12          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG12 | 12       | 0.12          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 12       | 0.12          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 12       | 0.12          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 12       | 0.12          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 12       | 0.12          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG11 | 23       | 0.12          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG12 | 23       | 0.12          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG13 | 23       | 0.12          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG11 | 23       | 0.12          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG12 | 23       | 0.12          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 23       | 0.12          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 23       | 0.12          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 23       | 0.12          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 23       | 0.12          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG11 | 37       | 0.12          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG12 | 37       | 0.12          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG13 | 37       | 0.12          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG11 | 37       | 0.12          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG12 | 37       | 0.12          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 37       | 0.12          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 37       | 0.12          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 37       | 0.12          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 37       | 0.12          |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 1        | 0.12          |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 1        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 1        | 0.12          |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 2        | 0.12          |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 2        | 0.12          |
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 2        | 0.12          |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 5        | 0.12          |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 5        | 0.12          |
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 5        | 0.12          |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 20       | 0.12          |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 20       | 0.12          |
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 20       | 0.12          |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 25       | 0.12          |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 25       | 0.12          |
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 25       | 0.12          |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 27       | 0.12          |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 27       | 0.12          |
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 27       | 0.12          |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 36       | 0.12          |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 36       | 0.12          |
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 36       | 0.12          |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 37       | 0.12          |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 37       | 0.12          |
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 37       | 0.12          |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 38       | 0.12          |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 38       | 0.12          |
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 38       | 0.12          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 12       | 0.12          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 12       | 0.12          |
| (1,1685) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 12       | 0.12          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 12       | 0.12          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 12       | 0.12          |
| (1,1685) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 12       | 0.12          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 12       | 0.12          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 12       | 0.12          |
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 12       | 0.12          |
| (1,1679) | 1:85:A:LEU:HD11 | 1:35:A:PHE:HD1  | 4        | 0.12          |
| (1,1679) | 1:85:A:LEU:HD11 | 1:35:A:PHE:HD2  | 4        | 0.12          |
| (1,1679) | 1:85:A:LEU:HD12 | 1:35:A:PHE:HD1  | 4        | 0.12          |
| (1,1679) | 1:85:A:LEU:HD12 | 1:35:A:PHE:HD2  | 4        | 0.12          |
| (1,1679) | 1:85:A:LEU:HD13 | 1:35:A:PHE:HD1  | 4        | 0.12          |
| (1,1679) | 1:85:A:LEU:HD13 | 1:35:A:PHE:HD2  | 4        | 0.12          |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 27       | 0.12          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 27       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 27       | 0.12          |
| (1,1653) | 1:81:A:VAL:HG11 | 1:31:A:CYS:HB2  | 5        | 0.12          |
| (1,1653) | 1:81:A:VAL:HG12 | 1:31:A:CYS:HB2  | 5        | 0.12          |
| (1,1653) | 1:81:A:VAL:HG13 | 1:31:A:CYS:HB2  | 5        | 0.12          |
| (1,1650) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 28       | 0.12          |
| (1,1650) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 28       | 0.12          |
| (1,1650) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 28       | 0.12          |
| (1,1650) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 28       | 0.12          |
| (1,1650) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 28       | 0.12          |
| (1,1650) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 28       | 0.12          |
| (1,1650) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 28       | 0.12          |
| (1,1650) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 28       | 0.12          |
| (1,1650) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 28       | 0.12          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 20       | 0.12          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 20       | 0.12          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 20       | 0.12          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 20       | 0.12          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 20       | 0.12          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 20       | 0.12          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 20       | 0.12          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 20       | 0.12          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 20       | 0.12          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 3        | 0.12          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 3        | 0.12          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 3        | 0.12          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 7        | 0.12          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 7        | 0.12          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 7        | 0.12          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 12       | 0.12          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 12       | 0.12          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 12       | 0.12          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 20       | 0.12          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 20       | 0.12          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 20       | 0.12          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 26       | 0.12          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 26       | 0.12          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 26       | 0.12          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 33       | 0.12          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 33       | 0.12          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H    | 33       | 0.12          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H    | 36       | 0.12          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H    | 36       | 0.12          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 36       | 0.12          |
| (1,1627) | 1:82:A:ILE:HG21 | 1:82:A:ILE:H   | 37       | 0.12          |
| (1,1627) | 1:82:A:ILE:HG22 | 1:82:A:ILE:H   | 37       | 0.12          |
| (1,1627) | 1:82:A:ILE:HG23 | 1:82:A:ILE:H   | 37       | 0.12          |
| (1,1624) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2 | 2        | 0.12          |
| (1,1624) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2 | 2        | 0.12          |
| (1,1624) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2 | 2        | 0.12          |
| (1,1622) | 1:82:A:ILE:HD11 | 1:83:A:ALA:H   | 8        | 0.12          |
| (1,1622) | 1:82:A:ILE:HD12 | 1:83:A:ALA:H   | 8        | 0.12          |
| (1,1622) | 1:82:A:ILE:HD13 | 1:83:A:ALA:H   | 8        | 0.12          |
| (1,1622) | 1:82:A:ILE:HD11 | 1:83:A:ALA:H   | 29       | 0.12          |
| (1,1622) | 1:82:A:ILE:HD12 | 1:83:A:ALA:H   | 29       | 0.12          |
| (1,1622) | 1:82:A:ILE:HD13 | 1:83:A:ALA:H   | 29       | 0.12          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2 | 13       | 0.12          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 13       | 0.12          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 13       | 0.12          |
| (1,1618) | 1:82:A:ILE:HD11 | 1:92:A:ARG:HD2 | 28       | 0.12          |
| (1,1618) | 1:82:A:ILE:HD12 | 1:92:A:ARG:HD2 | 28       | 0.12          |
| (1,1618) | 1:82:A:ILE:HD13 | 1:92:A:ARG:HD2 | 28       | 0.12          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 8        | 0.12          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 8        | 0.12          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 8        | 0.12          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 8        | 0.12          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 8        | 0.12          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 8        | 0.12          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 29       | 0.12          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 29       | 0.12          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 29       | 0.12          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 29       | 0.12          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 29       | 0.12          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 29       | 0.12          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1 | 33       | 0.12          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2 | 33       | 0.12          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1 | 33       | 0.12          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2 | 33       | 0.12          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1 | 33       | 0.12          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2 | 33       | 0.12          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 1        | 0.12          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 1        | 0.12          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 1        | 0.12          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 1        | 0.12          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 1        | 0.12          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 1        | 0.12          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 4        | 0.12          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 4        | 0.12          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 4        | 0.12          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 4        | 0.12          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 4        | 0.12          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 4        | 0.12          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 14       | 0.12          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 14       | 0.12          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 14       | 0.12          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 14       | 0.12          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 14       | 0.12          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 14       | 0.12          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 32       | 0.12          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 32       | 0.12          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 32       | 0.12          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 32       | 0.12          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 32       | 0.12          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 32       | 0.12          |
| (1,1550) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA   | 11       | 0.12          |
| (1,1550) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA   | 11       | 0.12          |
| (1,1550) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA   | 11       | 0.12          |
| (1,1550) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA   | 22       | 0.12          |
| (1,1550) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA   | 22       | 0.12          |
| (1,1550) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA   | 22       | 0.12          |
| (1,1550) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA   | 34       | 0.12          |
| (1,1550) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA   | 34       | 0.12          |
| (1,1550) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA   | 34       | 0.12          |
| (1,1514) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 6        | 0.12          |
| (1,1514) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 6        | 0.12          |
| (1,1514) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 6        | 0.12          |
| (1,1514) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 26       | 0.12          |
| (1,1514) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 26       | 0.12          |
| (1,1514) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 26       | 0.12          |
| (1,1514) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 29       | 0.12          |
| (1,1514) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 29       | 0.12          |
| (1,1514) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 29       | 0.12          |
| (1,1514) | 1:66:A:MET:HE1  | 1:66:A:MET:H   | 40       | 0.12          |
| (1,1514) | 1:66:A:MET:HE2  | 1:66:A:MET:H   | 40       | 0.12          |
| (1,1514) | 1:66:A:MET:HE3  | 1:66:A:MET:H   | 40       | 0.12          |
| (1,1513) | 1:66:A:MET:HE1  | 1:29:A:PHE:H   | 3        | 0.12          |
| (1,1513) | 1:66:A:MET:HE2  | 1:29:A:PHE:H   | 3        | 0.12          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1513) | 1:66:A:MET:HE3 | 1:29:A:PHE:H   | 3        | 0.12          |
| (1,1513) | 1:66:A:MET:HE1 | 1:29:A:PHE:H   | 18       | 0.12          |
| (1,1513) | 1:66:A:MET:HE2 | 1:29:A:PHE:H   | 18       | 0.12          |
| (1,1513) | 1:66:A:MET:HE3 | 1:29:A:PHE:H   | 18       | 0.12          |
| (1,1513) | 1:66:A:MET:HE1 | 1:29:A:PHE:H   | 32       | 0.12          |
| (1,1513) | 1:66:A:MET:HE2 | 1:29:A:PHE:H   | 32       | 0.12          |
| (1,1513) | 1:66:A:MET:HE3 | 1:29:A:PHE:H   | 32       | 0.12          |
| (1,1513) | 1:66:A:MET:HE1 | 1:29:A:PHE:H   | 34       | 0.12          |
| (1,1513) | 1:66:A:MET:HE2 | 1:29:A:PHE:H   | 34       | 0.12          |
| (1,1513) | 1:66:A:MET:HE3 | 1:29:A:PHE:H   | 34       | 0.12          |
| (1,1510) | 1:66:A:MET:HE1 | 1:42:A:TRP:HE1 | 7        | 0.12          |
| (1,1510) | 1:66:A:MET:HE2 | 1:42:A:TRP:HE1 | 7        | 0.12          |
| (1,1510) | 1:66:A:MET:HE3 | 1:42:A:TRP:HE1 | 7        | 0.12          |
| (1,1510) | 1:66:A:MET:HE1 | 1:42:A:TRP:HE1 | 10       | 0.12          |
| (1,1510) | 1:66:A:MET:HE2 | 1:42:A:TRP:HE1 | 10       | 0.12          |
| (1,1510) | 1:66:A:MET:HE3 | 1:42:A:TRP:HE1 | 10       | 0.12          |
| (1,1510) | 1:66:A:MET:HE1 | 1:42:A:TRP:HE1 | 34       | 0.12          |
| (1,1510) | 1:66:A:MET:HE2 | 1:42:A:TRP:HE1 | 34       | 0.12          |
| (1,1510) | 1:66:A:MET:HE3 | 1:42:A:TRP:HE1 | 34       | 0.12          |
| (1,1510) | 1:66:A:MET:HE1 | 1:42:A:TRP:HE1 | 38       | 0.12          |
| (1,1510) | 1:66:A:MET:HE2 | 1:42:A:TRP:HE1 | 38       | 0.12          |
| (1,1510) | 1:66:A:MET:HE3 | 1:42:A:TRP:HE1 | 38       | 0.12          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 6        | 0.12          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 6        | 0.12          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 6        | 0.12          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 6        | 0.12          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 6        | 0.12          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 6        | 0.12          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 15       | 0.12          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 15       | 0.12          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 15       | 0.12          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 15       | 0.12          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 15       | 0.12          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 15       | 0.12          |
| (1,1508) | 1:66:A:MET:HE1 | 1:42:A:TRP:HZ3 | 3        | 0.12          |
| (1,1508) | 1:66:A:MET:HE2 | 1:42:A:TRP:HZ3 | 3        | 0.12          |
| (1,1508) | 1:66:A:MET:HE3 | 1:42:A:TRP:HZ3 | 3        | 0.12          |
| (1,1508) | 1:66:A:MET:HE1 | 1:42:A:TRP:HZ3 | 26       | 0.12          |
| (1,1508) | 1:66:A:MET:HE2 | 1:42:A:TRP:HZ3 | 26       | 0.12          |
| (1,1508) | 1:66:A:MET:HE3 | 1:42:A:TRP:HZ3 | 26       | 0.12          |
| (1,1508) | 1:66:A:MET:HE1 | 1:42:A:TRP:HZ3 | 31       | 0.12          |
| (1,1508) | 1:66:A:MET:HE2 | 1:42:A:TRP:HZ3 | 31       | 0.12          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1508) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3 | 31       | 0.12          |
| (1,1508) | 1:66:A:MET:HE1  | 1:42:A:TRP:HZ3 | 32       | 0.12          |
| (1,1508) | 1:66:A:MET:HE2  | 1:42:A:TRP:HZ3 | 32       | 0.12          |
| (1,1508) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3 | 32       | 0.12          |
| (1,1507) | 1:66:A:MET:HE1  | 1:42:A:TRP:HB2 | 14       | 0.12          |
| (1,1507) | 1:66:A:MET:HE2  | 1:42:A:TRP:HB2 | 14       | 0.12          |
| (1,1507) | 1:66:A:MET:HE3  | 1:42:A:TRP:HB2 | 14       | 0.12          |
| (1,1507) | 1:66:A:MET:HE1  | 1:42:A:TRP:HB2 | 32       | 0.12          |
| (1,1507) | 1:66:A:MET:HE2  | 1:42:A:TRP:HB2 | 32       | 0.12          |
| (1,1507) | 1:66:A:MET:HE3  | 1:42:A:TRP:HB2 | 32       | 0.12          |
| (1,1507) | 1:66:A:MET:HE1  | 1:42:A:TRP:HB2 | 34       | 0.12          |
| (1,1507) | 1:66:A:MET:HE2  | 1:42:A:TRP:HB2 | 34       | 0.12          |
| (1,1507) | 1:66:A:MET:HE3  | 1:42:A:TRP:HB2 | 34       | 0.12          |
| (1,1503) | 1:66:A:MET:HE1  | 1:66:A:MET:HG2 | 2        | 0.12          |
| (1,1503) | 1:66:A:MET:HE2  | 1:66:A:MET:HG2 | 2        | 0.12          |
| (1,1503) | 1:66:A:MET:HE3  | 1:66:A:MET:HG2 | 2        | 0.12          |
| (1,1503) | 1:66:A:MET:HE1  | 1:66:A:MET:HG2 | 6        | 0.12          |
| (1,1503) | 1:66:A:MET:HE2  | 1:66:A:MET:HG2 | 6        | 0.12          |
| (1,1503) | 1:66:A:MET:HE3  | 1:66:A:MET:HG2 | 6        | 0.12          |
| (1,1503) | 1:66:A:MET:HE1  | 1:66:A:MET:HG2 | 7        | 0.12          |
| (1,1503) | 1:66:A:MET:HE2  | 1:66:A:MET:HG2 | 7        | 0.12          |
| (1,1503) | 1:66:A:MET:HE3  | 1:66:A:MET:HG2 | 7        | 0.12          |
| (1,1503) | 1:66:A:MET:HE1  | 1:66:A:MET:HG2 | 10       | 0.12          |
| (1,1503) | 1:66:A:MET:HE2  | 1:66:A:MET:HG2 | 10       | 0.12          |
| (1,1503) | 1:66:A:MET:HE3  | 1:66:A:MET:HG2 | 10       | 0.12          |
| (1,1503) | 1:66:A:MET:HE1  | 1:66:A:MET:HG2 | 12       | 0.12          |
| (1,1503) | 1:66:A:MET:HE2  | 1:66:A:MET:HG2 | 12       | 0.12          |
| (1,1503) | 1:66:A:MET:HE3  | 1:66:A:MET:HG2 | 12       | 0.12          |
| (1,1503) | 1:66:A:MET:HE1  | 1:66:A:MET:HG2 | 21       | 0.12          |
| (1,1503) | 1:66:A:MET:HE2  | 1:66:A:MET:HG2 | 21       | 0.12          |
| (1,1503) | 1:66:A:MET:HE3  | 1:66:A:MET:HG2 | 21       | 0.12          |
| (1,1503) | 1:66:A:MET:HE1  | 1:66:A:MET:HG2 | 24       | 0.12          |
| (1,1503) | 1:66:A:MET:HE2  | 1:66:A:MET:HG2 | 24       | 0.12          |
| (1,1503) | 1:66:A:MET:HE3  | 1:66:A:MET:HG2 | 24       | 0.12          |
| (1,1503) | 1:66:A:MET:HE1  | 1:66:A:MET:HG2 | 28       | 0.12          |
| (1,1503) | 1:66:A:MET:HE2  | 1:66:A:MET:HG2 | 28       | 0.12          |
| (1,1503) | 1:66:A:MET:HE3  | 1:66:A:MET:HG2 | 28       | 0.12          |
| (1,1503) | 1:66:A:MET:HE1  | 1:66:A:MET:HG2 | 40       | 0.12          |
| (1,1503) | 1:66:A:MET:HE2  | 1:66:A:MET:HG2 | 40       | 0.12          |
| (1,1503) | 1:66:A:MET:HE3  | 1:66:A:MET:HG2 | 40       | 0.12          |
| (1,1494) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ  | 1        | 0.12          |
| (1,1494) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ  | 1        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1494) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 1        | 0.12          |
| (1,1494) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 8        | 0.12          |
| (1,1494) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 8        | 0.12          |
| (1,1494) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 8        | 0.12          |
| (1,1494) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 16       | 0.12          |
| (1,1494) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 16       | 0.12          |
| (1,1494) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 16       | 0.12          |
| (1,1494) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 18       | 0.12          |
| (1,1494) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 18       | 0.12          |
| (1,1494) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 18       | 0.12          |
| (1,1494) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 21       | 0.12          |
| (1,1494) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 21       | 0.12          |
| (1,1494) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 21       | 0.12          |
| (1,1494) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 26       | 0.12          |
| (1,1494) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 26       | 0.12          |
| (1,1494) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 26       | 0.12          |
| (1,1494) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 28       | 0.12          |
| (1,1494) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 28       | 0.12          |
| (1,1494) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 28       | 0.12          |
| (1,1494) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 35       | 0.12          |
| (1,1494) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 35       | 0.12          |
| (1,1494) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 35       | 0.12          |
| (1,1494) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 36       | 0.12          |
| (1,1494) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 36       | 0.12          |
| (1,1494) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 36       | 0.12          |
| (1,1494) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 37       | 0.12          |
| (1,1494) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 37       | 0.12          |
| (1,1494) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 37       | 0.12          |
| (1,1494) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 40       | 0.12          |
| (1,1494) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 40       | 0.12          |
| (1,1494) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 40       | 0.12          |
| (1,1484) | 1:81:A:VAL:HB   | 1:42:A:TRP:HE1  | 17       | 0.12          |
| (1,1484) | 1:81:A:VAL:HB   | 1:42:A:TRP:HE1  | 18       | 0.12          |
| (1,1484) | 1:81:A:VAL:HB   | 1:42:A:TRP:HE1  | 20       | 0.12          |
| (1,1420) | 1:21:A:VAL:HG21 | 1:19:A:ILE:HD11 | 5        | 0.12          |
| (1,1420) | 1:21:A:VAL:HG21 | 1:19:A:ILE:HD12 | 5        | 0.12          |
| (1,1420) | 1:21:A:VAL:HG21 | 1:19:A:ILE:HD13 | 5        | 0.12          |
| (1,1420) | 1:21:A:VAL:HG22 | 1:19:A:ILE:HD11 | 5        | 0.12          |
| (1,1420) | 1:21:A:VAL:HG22 | 1:19:A:ILE:HD12 | 5        | 0.12          |
| (1,1420) | 1:21:A:VAL:HG22 | 1:19:A:ILE:HD13 | 5        | 0.12          |
| (1,1420) | 1:21:A:VAL:HG23 | 1:19:A:ILE:HD11 | 5        | 0.12          |
| (1,1420) | 1:21:A:VAL:HG23 | 1:19:A:ILE:HD12 | 5        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1420) | 1:21:A:VAL:HG23 | 1:19:A:ILE:HD13 | 5        | 0.12          |
| (1,1408) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HA  | 6        | 0.12          |
| (1,1408) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HA  | 6        | 0.12          |
| (1,1408) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HA  | 6        | 0.12          |
| (1,1403) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H    | 8        | 0.12          |
| (1,1403) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H    | 8        | 0.12          |
| (1,1403) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H    | 8        | 0.12          |
| (1,1403) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H    | 22       | 0.12          |
| (1,1403) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H    | 22       | 0.12          |
| (1,1403) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H    | 22       | 0.12          |
| (1,1403) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H    | 26       | 0.12          |
| (1,1403) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H    | 26       | 0.12          |
| (1,1403) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H    | 26       | 0.12          |
| (1,1401) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H    | 28       | 0.12          |
| (1,1401) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H    | 28       | 0.12          |
| (1,1401) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H    | 28       | 0.12          |
| (1,1400) | 1:95:A:ALA:HB1  | 1:16:A:ILE:HG12 | 19       | 0.12          |
| (1,1400) | 1:95:A:ALA:HB2  | 1:16:A:ILE:HG12 | 19       | 0.12          |
| (1,1400) | 1:95:A:ALA:HB3  | 1:16:A:ILE:HG12 | 19       | 0.12          |
| (1,1400) | 1:95:A:ALA:HB1  | 1:16:A:ILE:HG12 | 30       | 0.12          |
| (1,1400) | 1:95:A:ALA:HB2  | 1:16:A:ILE:HG12 | 30       | 0.12          |
| (1,1400) | 1:95:A:ALA:HB3  | 1:16:A:ILE:HG12 | 30       | 0.12          |
| (1,1387) | 1:91:A:ALA:HB1  | 1:12:A:PHE:HZ   | 12       | 0.12          |
| (1,1387) | 1:91:A:ALA:HB2  | 1:12:A:PHE:HZ   | 12       | 0.12          |
| (1,1387) | 1:91:A:ALA:HB3  | 1:12:A:PHE:HZ   | 12       | 0.12          |
| (1,1387) | 1:91:A:ALA:HB1  | 1:12:A:PHE:HZ   | 19       | 0.12          |
| (1,1387) | 1:91:A:ALA:HB2  | 1:12:A:PHE:HZ   | 19       | 0.12          |
| (1,1387) | 1:91:A:ALA:HB3  | 1:12:A:PHE:HZ   | 19       | 0.12          |
| (1,1387) | 1:91:A:ALA:HB1  | 1:12:A:PHE:HZ   | 24       | 0.12          |
| (1,1387) | 1:91:A:ALA:HB2  | 1:12:A:PHE:HZ   | 24       | 0.12          |
| (1,1387) | 1:91:A:ALA:HB3  | 1:12:A:PHE:HZ   | 24       | 0.12          |
| (1,1387) | 1:91:A:ALA:HB1  | 1:12:A:PHE:HZ   | 25       | 0.12          |
| (1,1387) | 1:91:A:ALA:HB2  | 1:12:A:PHE:HZ   | 25       | 0.12          |
| (1,1387) | 1:91:A:ALA:HB3  | 1:12:A:PHE:HZ   | 25       | 0.12          |
| (1,1387) | 1:91:A:ALA:HB1  | 1:12:A:PHE:HZ   | 40       | 0.12          |
| (1,1387) | 1:91:A:ALA:HB2  | 1:12:A:PHE:HZ   | 40       | 0.12          |
| (1,1387) | 1:91:A:ALA:HB3  | 1:12:A:PHE:HZ   | 40       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1  | 1:83:A:ALA:HB1  | 4        | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1  | 1:83:A:ALA:HB2  | 4        | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1  | 1:83:A:ALA:HB3  | 4        | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2  | 1:83:A:ALA:HB1  | 4        | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2  | 1:83:A:ALA:HB2  | 4        | 0.12          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 4        | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 4        | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 4        | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 4        | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 8        | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 8        | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 8        | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 8        | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 8        | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 8        | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 8        | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 8        | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 8        | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 10       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 10       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 10       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 10       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 10       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 10       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 10       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 10       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 10       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 12       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 12       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 12       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 12       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 12       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 12       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 12       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 12       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 12       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 17       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 17       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 17       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 17       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 17       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 17       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 17       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 17       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 17       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 21       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 21       | 0.12          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 21       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 21       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 21       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 21       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 21       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 21       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 21       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 23       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 23       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 23       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 23       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 23       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 23       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 23       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 23       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 23       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 27       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 27       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 27       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 27       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 27       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 27       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 27       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 27       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 27       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 28       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 28       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 28       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 28       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 28       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 28       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 28       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 28       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 28       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 29       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 29       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 29       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 29       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 29       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 29       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 29       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 29       | 0.12          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 29       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 32       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 32       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 32       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 32       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 32       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 32       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 32       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 32       | 0.12          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 32       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 4        | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 4        | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 4        | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 4        | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 4        | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 4        | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 4        | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 4        | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 4        | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 8        | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 8        | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 8        | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 8        | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 8        | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 8        | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 8        | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 8        | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 8        | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 10       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 10       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 10       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 10       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 10       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 10       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 10       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 10       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 10       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 12       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 12       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 12       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 12       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 12       | 0.12          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 12       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 12       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 12       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 12       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 17       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 17       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 17       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 17       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 17       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 17       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 17       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 17       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 17       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 21       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 21       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 21       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 21       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 21       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 21       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 21       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 21       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 21       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 23       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 23       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 23       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 23       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 23       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 23       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 23       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 23       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 23       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 27       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 27       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 27       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 27       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 27       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 27       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 27       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 27       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 27       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 28       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 28       | 0.12          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1379) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB3 | 28       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB1 | 28       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB2 | 28       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB3 | 28       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB1 | 28       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB2 | 28       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB3 | 28       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB1 | 29       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB2 | 29       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB3 | 29       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB1 | 29       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB2 | 29       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB3 | 29       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB1 | 29       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB2 | 29       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB3 | 29       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB1 | 32       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB2 | 32       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB3 | 32       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB1 | 32       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB2 | 32       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB3 | 32       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB1 | 32       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB2 | 32       | 0.12          |
| (1,1379) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB3 | 32       | 0.12          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3 | 7        | 0.12          |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3 | 24       | 0.12          |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 3        | 0.12          |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 3        | 0.12          |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 3        | 0.12          |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 4        | 0.12          |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 4        | 0.12          |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 4        | 0.12          |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 10       | 0.12          |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 10       | 0.12          |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 10       | 0.12          |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 19       | 0.12          |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 19       | 0.12          |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 19       | 0.12          |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H   | 20       | 0.12          |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 20       | 0.12          |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 20       | 0.12          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H  | 24       | 0.12          |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H  | 24       | 0.12          |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H  | 24       | 0.12          |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H  | 30       | 0.12          |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H  | 30       | 0.12          |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H  | 30       | 0.12          |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H  | 31       | 0.12          |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H  | 31       | 0.12          |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H  | 31       | 0.12          |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H  | 33       | 0.12          |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H  | 33       | 0.12          |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H  | 33       | 0.12          |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H  | 35       | 0.12          |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H  | 35       | 0.12          |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H  | 35       | 0.12          |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H  | 36       | 0.12          |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H  | 36       | 0.12          |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H  | 36       | 0.12          |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H  | 37       | 0.12          |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H  | 37       | 0.12          |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H  | 37       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 2        | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 2        | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 2        | 0.12          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 4        | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 4        | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 4        | 0.12          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 5        | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 5        | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 5        | 0.12          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 7        | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 7        | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 7        | 0.12          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 8        | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 8        | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 8        | 0.12          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 9        | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 9        | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 9        | 0.12          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 10       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 10       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 10       | 0.12          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 11       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 11       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 11       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 12       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 12       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 12       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 13       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 13       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 13       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 16       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 16       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 16       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 17       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 17       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 17       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 18       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 18       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 18       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 21       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 21       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 21       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 22       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 22       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 22       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 24       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 24       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 24       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 25       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 25       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 25       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 26       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 26       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 26       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 27       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 27       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 27       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 29       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 29       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 29       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 30       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 30       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 30       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA   | 31       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA   | 31       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA   | 31       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA   | 32       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA   | 32       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA   | 32       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA   | 33       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA   | 33       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA   | 33       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA   | 34       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA   | 34       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA   | 34       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA   | 35       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA   | 35       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA   | 35       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA   | 36       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA   | 36       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA   | 36       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA   | 37       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA   | 37       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA   | 37       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA   | 38       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA   | 38       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA   | 38       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA   | 39       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA   | 39       | 0.12          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA   | 39       | 0.12          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 18       | 0.12          |
| (1,1325) | 1:19:A:ILE:HB   | 1:20:A:VAL:H    | 34       | 0.12          |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 6        | 0.12          |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 12       | 0.12          |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 13       | 0.12          |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 16       | 0.12          |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 19       | 0.12          |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 23       | 0.12          |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 26       | 0.12          |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 31       | 0.12          |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 40       | 0.12          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 20       | 0.12          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 20       | 0.12          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 20       | 0.12          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 30       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 30       | 0.12          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 30       | 0.12          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1  | 6        | 0.12          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2  | 6        | 0.12          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3  | 6        | 0.12          |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1  | 6        | 0.12          |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2  | 6        | 0.12          |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3  | 6        | 0.12          |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1  | 6        | 0.12          |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2  | 6        | 0.12          |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3  | 6        | 0.12          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1  | 23       | 0.12          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2  | 23       | 0.12          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3  | 23       | 0.12          |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1  | 23       | 0.12          |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2  | 23       | 0.12          |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3  | 23       | 0.12          |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1  | 23       | 0.12          |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2  | 23       | 0.12          |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3  | 23       | 0.12          |
| (1,1289) | 1:40:A:VAL:HG21 | 1:42:A:TRP:HE1  | 29       | 0.12          |
| (1,1289) | 1:40:A:VAL:HG22 | 1:42:A:TRP:HE1  | 29       | 0.12          |
| (1,1289) | 1:40:A:VAL:HG23 | 1:42:A:TRP:HE1  | 29       | 0.12          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 20       | 0.12          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 20       | 0.12          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 20       | 0.12          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 30       | 0.12          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 30       | 0.12          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 30       | 0.12          |
| (1,1270) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3   | 16       | 0.12          |
| (1,1270) | 1:5:A:PHE:HB2   | 1:5:A:PHE:HB3   | 33       | 0.12          |
| (1,1269) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 16       | 0.12          |
| (1,1269) | 1:5:A:PHE:HB3   | 1:5:A:PHE:HB2   | 33       | 0.12          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 12       | 0.12          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 12       | 0.12          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 12       | 0.12          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 12       | 0.12          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 12       | 0.12          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 12       | 0.12          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 12       | 0.12          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 12       | 0.12          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 12       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 23       | 0.12          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 23       | 0.12          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 23       | 0.12          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 23       | 0.12          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 23       | 0.12          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 23       | 0.12          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 23       | 0.12          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 23       | 0.12          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 23       | 0.12          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 33       | 0.12          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 33       | 0.12          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 33       | 0.12          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 33       | 0.12          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 33       | 0.12          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 33       | 0.12          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 33       | 0.12          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 33       | 0.12          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 33       | 0.12          |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 17       | 0.12          |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 17       | 0.12          |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 17       | 0.12          |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 17       | 0.12          |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 17       | 0.12          |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 17       | 0.12          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 1        | 0.12          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 1        | 0.12          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 1        | 0.12          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 5        | 0.12          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 5        | 0.12          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 5        | 0.12          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 8        | 0.12          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 8        | 0.12          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 8        | 0.12          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 15       | 0.12          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 15       | 0.12          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 15       | 0.12          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 18       | 0.12          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 18       | 0.12          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 18       | 0.12          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 22       | 0.12          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 22       | 0.12          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 22       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 27       | 0.12          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 27       | 0.12          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 27       | 0.12          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 39       | 0.12          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 39       | 0.12          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 39       | 0.12          |
| (1,1261) | 1:67:A:THR:HG21 | 1:56:A:ASN:H    | 14       | 0.12          |
| (1,1261) | 1:67:A:THR:HG22 | 1:56:A:ASN:H    | 14       | 0.12          |
| (1,1261) | 1:67:A:THR:HG23 | 1:56:A:ASN:H    | 14       | 0.12          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 12       | 0.12          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 12       | 0.12          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 12       | 0.12          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 22       | 0.12          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 22       | 0.12          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 22       | 0.12          |
| (1,1239) | 1:13:A:THR:HG21 | 1:34:A:SER:H    | 3        | 0.12          |
| (1,1239) | 1:13:A:THR:HG22 | 1:34:A:SER:H    | 3        | 0.12          |
| (1,1239) | 1:13:A:THR:HG23 | 1:34:A:SER:H    | 3        | 0.12          |
| (1,1239) | 1:13:A:THR:HG21 | 1:34:A:SER:H    | 28       | 0.12          |
| (1,1239) | 1:13:A:THR:HG22 | 1:34:A:SER:H    | 28       | 0.12          |
| (1,1239) | 1:13:A:THR:HG23 | 1:34:A:SER:H    | 28       | 0.12          |
| (1,1239) | 1:13:A:THR:HG21 | 1:34:A:SER:H    | 39       | 0.12          |
| (1,1239) | 1:13:A:THR:HG22 | 1:34:A:SER:H    | 39       | 0.12          |
| (1,1239) | 1:13:A:THR:HG23 | 1:34:A:SER:H    | 39       | 0.12          |
| (1,1236) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3  | 22       | 0.12          |
| (1,1236) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3  | 22       | 0.12          |
| (1,1236) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3  | 22       | 0.12          |
| (1,1236) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3  | 31       | 0.12          |
| (1,1236) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3  | 31       | 0.12          |
| (1,1236) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3  | 31       | 0.12          |
| (1,1228) | 1:89:A:GLY:H    | 1:9:A:PRO:HG3   | 26       | 0.12          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 1        | 0.12          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 1        | 0.12          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 1        | 0.12          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 4        | 0.12          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 4        | 0.12          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 4        | 0.12          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 7        | 0.12          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 7        | 0.12          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 7        | 0.12          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 11       | 0.12          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 11       | 0.12          |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD23 | 11       | 0.12          |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD21 | 17       | 0.12          |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD22 | 17       | 0.12          |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD23 | 17       | 0.12          |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD21 | 23       | 0.12          |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD22 | 23       | 0.12          |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD23 | 23       | 0.12          |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD21 | 25       | 0.12          |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD22 | 25       | 0.12          |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD23 | 25       | 0.12          |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD21 | 29       | 0.12          |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD22 | 29       | 0.12          |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD23 | 29       | 0.12          |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD21 | 37       | 0.12          |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD22 | 37       | 0.12          |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD23 | 37       | 0.12          |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD21 | 39       | 0.12          |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD22 | 39       | 0.12          |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD23 | 39       | 0.12          |
| (1,1213) | 1:66:A:MET:H  | 1:28:A:THR:HA   | 6        | 0.12          |
| (1,1208) | 1:56:A:ASN:H  | 1:66:A:MET:HG2  | 1        | 0.12          |
| (1,1204) | 1:42:A:TRP:H  | 1:57:A:PHE:HE1  | 12       | 0.12          |
| (1,1204) | 1:42:A:TRP:H  | 1:57:A:PHE:HE2  | 12       | 0.12          |
| (1,1204) | 1:42:A:TRP:H  | 1:57:A:PHE:HE1  | 19       | 0.12          |
| (1,1204) | 1:42:A:TRP:H  | 1:57:A:PHE:HE2  | 19       | 0.12          |
| (1,1176) | 1:47:A:THR:H  | 1:44:A:LYS:HB3  | 14       | 0.12          |
| (1,1176) | 1:47:A:THR:H  | 1:44:A:LYS:HB3  | 15       | 0.12          |
| (1,1176) | 1:47:A:THR:H  | 1:44:A:LYS:HB3  | 16       | 0.12          |
| (1,1176) | 1:47:A:THR:H  | 1:44:A:LYS:HB3  | 23       | 0.12          |
| (1,1176) | 1:47:A:THR:H  | 1:44:A:LYS:HB3  | 39       | 0.12          |
| (1,1174) | 1:91:A:ALA:H  | 1:84:A:ARG:HA   | 35       | 0.12          |
| (1,1163) | 1:75:A:ASP:H  | 1:74:A:ASP:HB2  | 28       | 0.12          |
| (1,1149) | 1:54:A:LYS:H  | 1:53:A:GLN:HG3  | 20       | 0.12          |
| (1,1149) | 1:54:A:LYS:H  | 1:53:A:GLN:HG3  | 33       | 0.12          |
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 39       | 0.12          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 21       | 0.12          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 23       | 0.12          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 24       | 0.12          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 27       | 0.12          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 29       | 0.12          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 33       | 0.12          |
| (1,1095) | 1:74:A:ASP:H  | 1:73:A:PRO:HA   | 40       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1064) | 1:71:A:VAL:H    | 1:25:A:GLN:H    | 18       | 0.12          |
| (1,1064) | 1:71:A:VAL:H    | 1:25:A:GLN:H    | 39       | 0.12          |
| (1,1052) | 1:26:A:SER:H    | 1:25:A:GLN:HG2  | 11       | 0.12          |
| (1,1052) | 1:26:A:SER:H    | 1:25:A:GLN:HG2  | 14       | 0.12          |
| (1,1052) | 1:26:A:SER:H    | 1:25:A:GLN:HG2  | 15       | 0.12          |
| (1,1052) | 1:26:A:SER:H    | 1:25:A:GLN:HG2  | 25       | 0.12          |
| (1,1037) | 1:56:A:ASN:HD22 | 1:56:A:ASN:HA   | 32       | 0.12          |
| (1,1020) | 1:48:A:GLU:H    | 1:48:A:GLU:HG3  | 3        | 0.12          |
| (1,1020) | 1:48:A:GLU:H    | 1:48:A:GLU:HG3  | 7        | 0.12          |
| (1,1020) | 1:48:A:GLU:H    | 1:48:A:GLU:HG3  | 13       | 0.12          |
| (1,1020) | 1:48:A:GLU:H    | 1:48:A:GLU:HG3  | 24       | 0.12          |
| (1,1020) | 1:48:A:GLU:H    | 1:48:A:GLU:HG3  | 25       | 0.12          |
| (1,1020) | 1:48:A:GLU:H    | 1:48:A:GLU:HG3  | 32       | 0.12          |
| (1,1020) | 1:48:A:GLU:H    | 1:48:A:GLU:HG3  | 40       | 0.12          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG21 | 5        | 0.12          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG22 | 5        | 0.12          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG23 | 5        | 0.12          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG21 | 8        | 0.12          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG22 | 8        | 0.12          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG23 | 8        | 0.12          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG21 | 11       | 0.12          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG22 | 11       | 0.12          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG23 | 11       | 0.12          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG21 | 12       | 0.12          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG22 | 12       | 0.12          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG23 | 12       | 0.12          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG21 | 14       | 0.12          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG22 | 14       | 0.12          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG23 | 14       | 0.12          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG21 | 24       | 0.12          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG22 | 24       | 0.12          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG23 | 24       | 0.12          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG21 | 27       | 0.12          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG22 | 27       | 0.12          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG23 | 27       | 0.12          |
| (1,987)  | 1:12:A:PHE:H    | 1:11:A:GLN:HB2  | 11       | 0.12          |
| (1,987)  | 1:12:A:PHE:H    | 1:11:A:GLN:HB2  | 12       | 0.12          |
| (1,987)  | 1:12:A:PHE:H    | 1:11:A:GLN:HB2  | 26       | 0.12          |
| (1,987)  | 1:12:A:PHE:H    | 1:11:A:GLN:HB2  | 36       | 0.12          |
| (1,978)  | 1:20:A:VAL:H    | 1:19:A:ILE:HB   | 18       | 0.12          |
| (1,978)  | 1:20:A:VAL:H    | 1:19:A:ILE:HB   | 34       | 0.12          |
| (1,971)  | 1:21:A:VAL:H    | 1:21:A:VAL:HG21 | 7        | 0.12          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,971) | 1:21:A:VAL:H | 1:21:A:VAL:HG22 | 7        | 0.12          |
| (1,971) | 1:21:A:VAL:H | 1:21:A:VAL:HG23 | 7        | 0.12          |
| (1,971) | 1:21:A:VAL:H | 1:21:A:VAL:HG21 | 34       | 0.12          |
| (1,971) | 1:21:A:VAL:H | 1:21:A:VAL:HG22 | 34       | 0.12          |
| (1,971) | 1:21:A:VAL:H | 1:21:A:VAL:HG23 | 34       | 0.12          |
| (1,967) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 2        | 0.12          |
| (1,967) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 4        | 0.12          |
| (1,967) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 20       | 0.12          |
| (1,967) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 22       | 0.12          |
| (1,967) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 25       | 0.12          |
| (1,967) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 31       | 0.12          |
| (1,967) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 40       | 0.12          |
| (1,941) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 10       | 0.12          |
| (1,941) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 37       | 0.12          |
| (1,941) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 39       | 0.12          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 13       | 0.12          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 13       | 0.12          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 13       | 0.12          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 24       | 0.12          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 24       | 0.12          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 24       | 0.12          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 26       | 0.12          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 26       | 0.12          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 26       | 0.12          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 28       | 0.12          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 28       | 0.12          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 28       | 0.12          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 30       | 0.12          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 30       | 0.12          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 30       | 0.12          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 31       | 0.12          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 31       | 0.12          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 31       | 0.12          |
| (1,932) | 1:98:A:LYS:H | 1:19:A:ILE:HB   | 14       | 0.12          |
| (1,915) | 1:37:A:ASP:H | 1:37:A:ASP:HA   | 18       | 0.12          |
| (1,899) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 1        | 0.12          |
| (1,899) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 8        | 0.12          |
| (1,899) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 9        | 0.12          |
| (1,899) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 12       | 0.12          |
| (1,899) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 14       | 0.12          |
| (1,899) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 39       | 0.12          |
| (1,889) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 35       | 0.12          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,863) | 1:86:A:GLU:H | 1:85:A:LEU:HB3  | 22       | 0.12          |
| (1,863) | 1:86:A:GLU:H | 1:85:A:LEU:HB3  | 37       | 0.12          |
| (1,863) | 1:86:A:GLU:H | 1:85:A:LEU:HB3  | 38       | 0.12          |
| (1,863) | 1:86:A:GLU:H | 1:85:A:LEU:HB3  | 40       | 0.12          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 2        | 0.12          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 2        | 0.12          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 2        | 0.12          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 13       | 0.12          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 13       | 0.12          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 13       | 0.12          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 23       | 0.12          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 23       | 0.12          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 23       | 0.12          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 35       | 0.12          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 35       | 0.12          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 35       | 0.12          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 18       | 0.12          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 18       | 0.12          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 18       | 0.12          |
| (1,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB   | 1        | 0.12          |
| (1,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB   | 2        | 0.12          |
| (1,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB   | 3        | 0.12          |
| (1,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB   | 30       | 0.12          |
| (1,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB   | 32       | 0.12          |
| (1,726) | 1:49:A:LEU:H | 1:48:A:GLU:HG3  | 10       | 0.12          |
| (1,726) | 1:49:A:LEU:H | 1:48:A:GLU:HG3  | 16       | 0.12          |
| (1,726) | 1:49:A:LEU:H | 1:48:A:GLU:HG3  | 23       | 0.12          |
| (1,726) | 1:49:A:LEU:H | 1:48:A:GLU:HG3  | 24       | 0.12          |
| (1,726) | 1:49:A:LEU:H | 1:48:A:GLU:HG3  | 25       | 0.12          |
| (1,726) | 1:49:A:LEU:H | 1:48:A:GLU:HG3  | 40       | 0.12          |
| (1,709) | 1:16:A:ILE:H | 1:31:A:CYS:HB2  | 21       | 0.12          |
| (1,709) | 1:16:A:ILE:H | 1:31:A:CYS:HB2  | 34       | 0.12          |
| (1,683) | 1:23:A:GLU:H | 1:22:A:SER:HB3  | 7        | 0.12          |
| (1,672) | 1:72:A:THR:H | 1:73:A:PRO:HD2  | 17       | 0.12          |
| (1,666) | 1:72:A:THR:H | 1:72:A:THR:HB   | 1        | 0.12          |
| (1,666) | 1:72:A:THR:H | 1:72:A:THR:HB   | 7        | 0.12          |
| (1,666) | 1:72:A:THR:H | 1:72:A:THR:HB   | 10       | 0.12          |
| (1,666) | 1:72:A:THR:H | 1:72:A:THR:HB   | 19       | 0.12          |
| (1,666) | 1:72:A:THR:H | 1:72:A:THR:HB   | 28       | 0.12          |
| (1,661) | 1:7:A:ALA:H  | 1:6:A:THR:HA    | 5        | 0.12          |
| (1,661) | 1:7:A:ALA:H  | 1:6:A:THR:HA    | 10       | 0.12          |
| (1,661) | 1:7:A:ALA:H  | 1:6:A:THR:HA    | 31       | 0.12          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 12       | 0.12          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 13       | 0.12          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 18       | 0.12          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 20       | 0.12          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 30       | 0.12          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 35       | 0.12          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 36       | 0.12          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 37       | 0.12          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 14       | 0.12          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 16       | 0.12          |
| (1,609) | 1:43:A:TYR:H  | 1:42:A:TRP:HB2  | 12       | 0.12          |
| (1,609) | 1:43:A:TYR:H  | 1:42:A:TRP:HB2  | 19       | 0.12          |
| (1,609) | 1:43:A:TYR:H  | 1:42:A:TRP:HB2  | 29       | 0.12          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 1        | 0.12          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 1        | 0.12          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 1        | 0.12          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 3        | 0.12          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 3        | 0.12          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 3        | 0.12          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 4        | 0.12          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 4        | 0.12          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 4        | 0.12          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 7        | 0.12          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 7        | 0.12          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 7        | 0.12          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 12       | 0.12          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 12       | 0.12          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 12       | 0.12          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 13       | 0.12          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 13       | 0.12          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 13       | 0.12          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 15       | 0.12          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 15       | 0.12          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 15       | 0.12          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 16       | 0.12          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 16       | 0.12          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 16       | 0.12          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 27       | 0.12          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 27       | 0.12          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 27       | 0.12          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 32       | 0.12          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 32       | 0.12          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 32       | 0.12          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 33       | 0.12          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 33       | 0.12          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 33       | 0.12          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 37       | 0.12          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 37       | 0.12          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 37       | 0.12          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 38       | 0.12          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 38       | 0.12          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 38       | 0.12          |
| (1,560) | 1:47:A:THR:H | 1:47:A:THR:HA   | 11       | 0.12          |
| (1,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1  | 12       | 0.12          |
| (1,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2  | 12       | 0.12          |
| (1,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1  | 31       | 0.12          |
| (1,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2  | 31       | 0.12          |
| (1,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1  | 36       | 0.12          |
| (1,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2  | 36       | 0.12          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 11       | 0.12          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 11       | 0.12          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 11       | 0.12          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 16       | 0.12          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 16       | 0.12          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 16       | 0.12          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 18       | 0.12          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 18       | 0.12          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 18       | 0.12          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 20       | 0.12          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 20       | 0.12          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 20       | 0.12          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 23       | 0.12          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 23       | 0.12          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 23       | 0.12          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 27       | 0.12          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 27       | 0.12          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 27       | 0.12          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 29       | 0.12          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 29       | 0.12          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 29       | 0.12          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 33       | 0.12          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 33       | 0.12          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 33       | 0.12          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 35       | 0.12          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 35       | 0.12          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 35       | 0.12          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 40       | 0.12          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 40       | 0.12          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 40       | 0.12          |
| (1,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 2        | 0.12          |
| (1,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 7        | 0.12          |
| (1,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 25       | 0.12          |
| (1,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 27       | 0.12          |
| (1,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 30       | 0.12          |
| (1,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 32       | 0.12          |
| (1,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 36       | 0.12          |
| (1,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 40       | 0.12          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 1        | 0.12          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 4        | 0.12          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 7        | 0.12          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 8        | 0.12          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 12       | 0.12          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 13       | 0.12          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 14       | 0.12          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 16       | 0.12          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 20       | 0.12          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 21       | 0.12          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 22       | 0.12          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 23       | 0.12          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 24       | 0.12          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 25       | 0.12          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 26       | 0.12          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 27       | 0.12          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 30       | 0.12          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 31       | 0.12          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 32       | 0.12          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 33       | 0.12          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 35       | 0.12          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 36       | 0.12          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 37       | 0.12          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 38       | 0.12          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 40       | 0.12          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 2        | 0.12          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 8        | 0.12          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 5        | 0.12          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 9        | 0.12          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 14       | 0.12          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 15       | 0.12          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 34       | 0.12          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 19       | 0.12          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 21       | 0.12          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 28       | 0.12          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 29       | 0.12          |
| (1,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 20       | 0.12          |
| (1,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 26       | 0.12          |
| (1,488) | 1:19:A:ILE:H | 1:18:A:ASN:HB3  | 27       | 0.12          |
| (1,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD21 | 7        | 0.12          |
| (1,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD22 | 7        | 0.12          |
| (1,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD23 | 7        | 0.12          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 5        | 0.12          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 14       | 0.12          |
| (1,403) | 1:77:A:GLY:H | 1:76:A:GLU:HB2  | 17       | 0.12          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 6        | 0.12          |
| (1,394) | 1:77:A:GLY:H | 1:97:A:LEU:HA   | 15       | 0.12          |
| (1,393) | 1:77:A:GLY:H | 1:96:A:GLU:HA   | 19       | 0.12          |
| (1,393) | 1:77:A:GLY:H | 1:96:A:GLU:HA   | 37       | 0.12          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD11 | 2        | 0.12          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD12 | 2        | 0.12          |
| (1,373) | 1:97:A:LEU:H | 1:97:A:LEU:HD13 | 2        | 0.12          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 8        | 0.12          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 8        | 0.12          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 8        | 0.12          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 22       | 0.12          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 22       | 0.12          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 22       | 0.12          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 26       | 0.12          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 26       | 0.12          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 26       | 0.12          |
| (1,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 6        | 0.12          |
| (1,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 7        | 0.12          |
| (1,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 10       | 0.12          |
| (1,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 15       | 0.12          |
| (1,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 17       | 0.12          |
| (1,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 22       | 0.12          |
| (1,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 23       | 0.12          |
| (1,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD1  | 7        | 0.12          |
| (1,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD2  | 7        | 0.12          |
| (1,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD1  | 10       | 0.12          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD2  | 10       | 0.12          |
| (1,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD1  | 33       | 0.12          |
| (1,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD2  | 33       | 0.12          |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 3        | 0.12          |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 4        | 0.12          |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 21       | 0.12          |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 24       | 0.12          |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 39       | 0.12          |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 40       | 0.12          |
| (1,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3  | 5        | 0.12          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 17       | 0.12          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 17       | 0.12          |
| (1,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 17       | 0.12          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 2        | 0.12          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 6        | 0.12          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 7        | 0.12          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 9        | 0.12          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 11       | 0.12          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 19       | 0.12          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 20       | 0.12          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 21       | 0.12          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 23       | 0.12          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 25       | 0.12          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 27       | 0.12          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 33       | 0.12          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 38       | 0.12          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 39       | 0.12          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1  | 2        | 0.12          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2  | 2        | 0.12          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1  | 5        | 0.12          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2  | 5        | 0.12          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1  | 10       | 0.12          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2  | 10       | 0.12          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1  | 23       | 0.12          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2  | 23       | 0.12          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1  | 29       | 0.12          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2  | 29       | 0.12          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1  | 30       | 0.12          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2  | 30       | 0.12          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1  | 36       | 0.12          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2  | 36       | 0.12          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1  | 37       | 0.12          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,230)  | 1:13:A:THR:H   | 1:12:A:PHE:HD2  | 37       | 0.12          |
| (1,201)  | 1:90:A:GLU:H   | 1:89:A:GLY:HA2  | 13       | 0.12          |
| (1,201)  | 1:90:A:GLU:H   | 1:89:A:GLY:HA2  | 17       | 0.12          |
| (1,201)  | 1:90:A:GLU:H   | 1:89:A:GLY:HA2  | 21       | 0.12          |
| (1,201)  | 1:90:A:GLU:H   | 1:89:A:GLY:HA2  | 24       | 0.12          |
| (1,201)  | 1:90:A:GLU:H   | 1:89:A:GLY:HA2  | 25       | 0.12          |
| (1,201)  | 1:90:A:GLU:H   | 1:89:A:GLY:HA2  | 30       | 0.12          |
| (1,201)  | 1:90:A:GLU:H   | 1:89:A:GLY:HA2  | 35       | 0.12          |
| (1,201)  | 1:90:A:GLU:H   | 1:89:A:GLY:HA2  | 40       | 0.12          |
| (1,199)  | 1:90:A:GLU:H   | 1:10:A:ILE:HG21 | 25       | 0.12          |
| (1,199)  | 1:90:A:GLU:H   | 1:10:A:ILE:HG22 | 25       | 0.12          |
| (1,199)  | 1:90:A:GLU:H   | 1:10:A:ILE:HG23 | 25       | 0.12          |
| (1,199)  | 1:90:A:GLU:H   | 1:10:A:ILE:HG21 | 30       | 0.12          |
| (1,199)  | 1:90:A:GLU:H   | 1:10:A:ILE:HG22 | 30       | 0.12          |
| (1,199)  | 1:90:A:GLU:H   | 1:10:A:ILE:HG23 | 30       | 0.12          |
| (1,199)  | 1:90:A:GLU:H   | 1:10:A:ILE:HG21 | 34       | 0.12          |
| (1,199)  | 1:90:A:GLU:H   | 1:10:A:ILE:HG22 | 34       | 0.12          |
| (1,199)  | 1:90:A:GLU:H   | 1:10:A:ILE:HG23 | 34       | 0.12          |
| (1,165)  | 1:10:A:ILE:H   | 1:9:A:PRO:HB2   | 16       | 0.12          |
| (1,165)  | 1:10:A:ILE:H   | 1:9:A:PRO:HB2   | 20       | 0.12          |
| (1,148)  | 1:45:A:GLY:H   | 1:46:A:PRO:HD2  | 22       | 0.12          |
| (1,148)  | 1:45:A:GLY:H   | 1:46:A:PRO:HD2  | 35       | 0.12          |
| (1,139)  | 1:101:A:LEU:H  | 1:100:A:GLU:H   | 39       | 0.12          |
| (1,111)  | 1:63:A:CYS:H   | 1:60:A:ASP:H    | 3        | 0.12          |
| (1,111)  | 1:63:A:CYS:H   | 1:60:A:ASP:H    | 26       | 0.12          |
| (1,37)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3  | 25       | 0.12          |
| (1,37)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3  | 26       | 0.12          |
| (1,37)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3  | 27       | 0.12          |
| (1,37)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3  | 32       | 0.12          |
| (1,37)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3  | 33       | 0.12          |
| (1,37)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3  | 37       | 0.12          |
| (1,37)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3  | 39       | 0.12          |
| (1,35)   | 1:88:A:ARG:H   | 1:88:A:ARG:HG2  | 2        | 0.12          |
| (1,35)   | 1:88:A:ARG:H   | 1:88:A:ARG:HG2  | 4        | 0.12          |
| (1,35)   | 1:88:A:ARG:H   | 1:88:A:ARG:HG2  | 18       | 0.12          |
| (1,25)   | 1:89:A:GLY:H   | 1:88:A:ARG:HB3  | 6        | 0.12          |
| (1,25)   | 1:89:A:GLY:H   | 1:88:A:ARG:HB3  | 9        | 0.12          |
| (3,3217) | 1:69:A:HIS:HE1 | 1:67:A:THR:HB   | 24       | 0.11          |
| (3,3217) | 1:69:A:HIS:HE1 | 1:67:A:THR:HB   | 28       | 0.11          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 5        | 0.11          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 5        | 0.11          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 11       | 0.11          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 11       | 0.11          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 13       | 0.11          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 13       | 0.11          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 20       | 0.11          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 20       | 0.11          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 23       | 0.11          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 23       | 0.11          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 26       | 0.11          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 26       | 0.11          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 30       | 0.11          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 30       | 0.11          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 31       | 0.11          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 31       | 0.11          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 37       | 0.11          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 37       | 0.11          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 25       | 0.11          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 25       | 0.11          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 25       | 0.11          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 25       | 0.11          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 25       | 0.11          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 25       | 0.11          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 32       | 0.11          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 32       | 0.11          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 32       | 0.11          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 32       | 0.11          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 32       | 0.11          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 32       | 0.11          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 34       | 0.11          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 34       | 0.11          |
| (3,3206) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 34       | 0.11          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 34       | 0.11          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 34       | 0.11          |
| (3,3206) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 34       | 0.11          |
| (3,3203) | 1:42:A:TRP:HZ2 | 1:30:A:GLU:HA   | 1        | 0.11          |
| (3,3203) | 1:42:A:TRP:HZ2 | 1:30:A:GLU:HA   | 18       | 0.11          |
| (3,3203) | 1:42:A:TRP:HZ2 | 1:30:A:GLU:HA   | 28       | 0.11          |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG21 | 9        | 0.11          |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG22 | 9        | 0.11          |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG23 | 9        | 0.11          |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG21 | 22       | 0.11          |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG22 | 22       | 0.11          |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG23 | 22       | 0.11          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1 | 13       | 0.11          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2 | 13       | 0.11          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1 | 13       | 0.11          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2 | 13       | 0.11          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1 | 14       | 0.11          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2 | 14       | 0.11          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1 | 14       | 0.11          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2 | 14       | 0.11          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1 | 34       | 0.11          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2 | 34       | 0.11          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1 | 34       | 0.11          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2 | 34       | 0.11          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1 | 37       | 0.11          |
| (3,3196) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2 | 37       | 0.11          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1 | 37       | 0.11          |
| (3,3196) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2 | 37       | 0.11          |
| (3,3191) | 1:43:A:TYR:HD1 | 1:44:A:LYS:H   | 31       | 0.11          |
| (3,3191) | 1:43:A:TYR:HD2 | 1:44:A:LYS:H   | 31       | 0.11          |
| (3,3183) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB  | 29       | 0.11          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1 | 2        | 0.11          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2 | 2        | 0.11          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3 | 2        | 0.11          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1 | 4        | 0.11          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2 | 4        | 0.11          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3 | 4        | 0.11          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1 | 14       | 0.11          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2 | 14       | 0.11          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3 | 14       | 0.11          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1 | 23       | 0.11          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2 | 23       | 0.11          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3 | 23       | 0.11          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1 | 24       | 0.11          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2 | 24       | 0.11          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3 | 24       | 0.11          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1 | 32       | 0.11          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2 | 32       | 0.11          |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3 | 32       | 0.11          |
| (3,3175) | 1:69:A:HIS:HD2 | 1:69:A:HIS:HB3 | 14       | 0.11          |
| (3,3164) | 1:42:A:TRP:HD1 | 1:41:A:THR:HA  | 39       | 0.11          |
| (3,3143) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3 | 10       | 0.11          |
| (3,3143) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3 | 10       | 0.11          |
| (3,3143) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3 | 14       | 0.11          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3143) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 14       | 0.11          |
| (3,3143) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3  | 18       | 0.11          |
| (3,3143) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 18       | 0.11          |
| (3,3143) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3  | 26       | 0.11          |
| (3,3143) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 26       | 0.11          |
| (3,3143) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3  | 38       | 0.11          |
| (3,3143) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 38       | 0.11          |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2  | 1        | 0.11          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2  | 1        | 0.11          |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2  | 3        | 0.11          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2  | 3        | 0.11          |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2  | 5        | 0.11          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2  | 5        | 0.11          |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2  | 13       | 0.11          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2  | 13       | 0.11          |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2  | 22       | 0.11          |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2  | 22       | 0.11          |
| (3,3139) | 1:65:A:TYR:HE1 | 1:60:A:ASP:HB3  | 20       | 0.11          |
| (3,3139) | 1:65:A:TYR:HE2 | 1:60:A:ASP:HB3  | 20       | 0.11          |
| (3,3139) | 1:65:A:TYR:HE1 | 1:60:A:ASP:HB3  | 30       | 0.11          |
| (3,3139) | 1:65:A:TYR:HE2 | 1:60:A:ASP:HB3  | 30       | 0.11          |
| (3,3139) | 1:65:A:TYR:HE1 | 1:60:A:ASP:HB3  | 33       | 0.11          |
| (3,3139) | 1:65:A:TYR:HE2 | 1:60:A:ASP:HB3  | 33       | 0.11          |
| (3,3138) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB2  | 30       | 0.11          |
| (3,3138) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB2  | 30       | 0.11          |
| (3,3137) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3  | 31       | 0.11          |
| (3,3137) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3  | 31       | 0.11          |
| (3,3137) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3  | 40       | 0.11          |
| (3,3137) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3  | 40       | 0.11          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 6        | 0.11          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 6        | 0.11          |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 6        | 0.11          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 6        | 0.11          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 6        | 0.11          |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 6        | 0.11          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 3        | 0.11          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 3        | 0.11          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 3        | 0.11          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 3        | 0.11          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 3        | 0.11          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 3        | 0.11          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 5        | 0.11          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 5        | 0.11          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 5        | 0.11          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 5        | 0.11          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 5        | 0.11          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 5        | 0.11          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 10       | 0.11          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 10       | 0.11          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 10       | 0.11          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 10       | 0.11          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 10       | 0.11          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 10       | 0.11          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 19       | 0.11          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 19       | 0.11          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 19       | 0.11          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 19       | 0.11          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 19       | 0.11          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 19       | 0.11          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 21       | 0.11          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 21       | 0.11          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 21       | 0.11          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 21       | 0.11          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 21       | 0.11          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 21       | 0.11          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 33       | 0.11          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 33       | 0.11          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 33       | 0.11          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 33       | 0.11          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 33       | 0.11          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 33       | 0.11          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 40       | 0.11          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 40       | 0.11          |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 40       | 0.11          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 40       | 0.11          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 40       | 0.11          |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 40       | 0.11          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 5        | 0.11          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 5        | 0.11          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 5        | 0.11          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 5        | 0.11          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 30       | 0.11          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 30       | 0.11          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 30       | 0.11          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2 | 30       | 0.11          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1 | 33       | 0.11          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2 | 33       | 0.11          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1 | 33       | 0.11          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2 | 33       | 0.11          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1 | 35       | 0.11          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2 | 35       | 0.11          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1 | 35       | 0.11          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2 | 35       | 0.11          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1 | 38       | 0.11          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2 | 38       | 0.11          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1 | 38       | 0.11          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2 | 38       | 0.11          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1 | 40       | 0.11          |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2 | 40       | 0.11          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1 | 40       | 0.11          |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2 | 40       | 0.11          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1 | 2        | 0.11          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2 | 2        | 0.11          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1 | 2        | 0.11          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2 | 2        | 0.11          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1 | 2        | 0.11          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2 | 2        | 0.11          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1 | 18       | 0.11          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2 | 18       | 0.11          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1 | 18       | 0.11          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2 | 18       | 0.11          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1 | 18       | 0.11          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2 | 18       | 0.11          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1 | 30       | 0.11          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2 | 30       | 0.11          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1 | 30       | 0.11          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2 | 30       | 0.11          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1 | 30       | 0.11          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2 | 30       | 0.11          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1 | 34       | 0.11          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2 | 34       | 0.11          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1 | 34       | 0.11          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2 | 34       | 0.11          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1 | 34       | 0.11          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2 | 34       | 0.11          |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1 | 38       | 0.11          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 38       | 0.11          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 38       | 0.11          |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 38       | 0.11          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 38       | 0.11          |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 38       | 0.11          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 9        | 0.11          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 9        | 0.11          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 9        | 0.11          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 12       | 0.11          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 12       | 0.11          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 12       | 0.11          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 21       | 0.11          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 21       | 0.11          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 21       | 0.11          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 22       | 0.11          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 22       | 0.11          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 22       | 0.11          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 38       | 0.11          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 38       | 0.11          |
| (3,3090) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 38       | 0.11          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 16       | 0.11          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 16       | 0.11          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 18       | 0.11          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 18       | 0.11          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 36       | 0.11          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 36       | 0.11          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 40       | 0.11          |
| (3,3088) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 40       | 0.11          |
| (3,3048) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG21 | 7        | 0.11          |
| (3,3048) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG22 | 7        | 0.11          |
| (3,3048) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG23 | 7        | 0.11          |
| (3,3048) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG21 | 14       | 0.11          |
| (3,3048) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG22 | 14       | 0.11          |
| (3,3048) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG23 | 14       | 0.11          |
| (3,3041) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE1  | 1        | 0.11          |
| (3,3041) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE2  | 1        | 0.11          |
| (3,3041) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE1  | 6        | 0.11          |
| (3,3041) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE2  | 6        | 0.11          |
| (3,3041) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE1  | 18       | 0.11          |
| (3,3041) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE2  | 18       | 0.11          |
| (3,3041) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE1  | 27       | 0.11          |
| (3,3041) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE2  | 27       | 0.11          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 5        | 0.11          |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 5        | 0.11          |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 13       | 0.11          |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 13       | 0.11          |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 17       | 0.11          |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 17       | 0.11          |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 21       | 0.11          |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 21       | 0.11          |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 33       | 0.11          |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 33       | 0.11          |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 35       | 0.11          |
| (3,3021) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 35       | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 6        | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 6        | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 6        | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 9        | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 9        | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 9        | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 10       | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 10       | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 10       | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 15       | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 15       | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 15       | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 16       | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 16       | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 16       | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 17       | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 17       | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 17       | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 20       | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 20       | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 20       | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 21       | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 21       | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 21       | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 24       | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 24       | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 24       | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 29       | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 29       | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 29       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,3020) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG21 | 33       | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG22 | 33       | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG23 | 33       | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG21 | 39       | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG22 | 39       | 0.11          |
| (3,3020) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG23 | 39       | 0.11          |
| (3,3017) | 1:102:A:ARG:HD3 | 1:102:A:ARG:HB2 | 24       | 0.11          |
| (3,3017) | 1:102:A:ARG:HD3 | 1:102:A:ARG:HB2 | 28       | 0.11          |
| (3,3017) | 1:102:A:ARG:HD3 | 1:102:A:ARG:HB2 | 30       | 0.11          |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG21 | 12       | 0.11          |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG22 | 12       | 0.11          |
| (3,3012) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG23 | 12       | 0.11          |
| (3,3004) | 1:15:A:ARG:HG2  | 1:93:A:SER:HB3  | 3        | 0.11          |
| (3,3004) | 1:15:A:ARG:HG2  | 1:93:A:SER:HB3  | 29       | 0.11          |
| (3,3004) | 1:15:A:ARG:HG2  | 1:93:A:SER:HB3  | 34       | 0.11          |
| (3,3004) | 1:15:A:ARG:HG2  | 1:93:A:SER:HB3  | 37       | 0.11          |
| (3,2982) | 1:65:A:TYR:HA   | 1:42:A:TRP:HZ2  | 6        | 0.11          |
| (3,2982) | 1:65:A:TYR:HA   | 1:42:A:TRP:HZ2  | 9        | 0.11          |
| (3,2982) | 1:65:A:TYR:HA   | 1:42:A:TRP:HZ2  | 30       | 0.11          |
| (3,2982) | 1:65:A:TYR:HA   | 1:42:A:TRP:HZ2  | 35       | 0.11          |
| (3,2982) | 1:65:A:TYR:HA   | 1:42:A:TRP:HZ2  | 38       | 0.11          |
| (3,2957) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 9        | 0.11          |
| (3,2957) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 12       | 0.11          |
| (3,2957) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 27       | 0.11          |
| (3,2957) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 40       | 0.11          |
| (3,2949) | 1:90:A:GLU:HA   | 1:84:A:ARG:HA   | 4        | 0.11          |
| (3,2949) | 1:90:A:GLU:HA   | 1:84:A:ARG:HA   | 8        | 0.11          |
| (3,2944) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD1  | 10       | 0.11          |
| (3,2944) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD2  | 10       | 0.11          |
| (3,2944) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD1  | 14       | 0.11          |
| (3,2944) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD2  | 14       | 0.11          |
| (3,2944) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD1  | 18       | 0.11          |
| (3,2944) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD2  | 18       | 0.11          |
| (3,2944) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD1  | 26       | 0.11          |
| (3,2944) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD2  | 26       | 0.11          |
| (3,2944) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD1  | 38       | 0.11          |
| (3,2944) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD2  | 38       | 0.11          |
| (3,2938) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 6        | 0.11          |
| (3,2938) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 10       | 0.11          |
| (3,2938) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 21       | 0.11          |
| (3,2938) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 28       | 0.11          |
| (3,2938) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 37       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2938) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 40       | 0.11          |
| (3,2917) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HG3  | 6        | 0.11          |
| (3,2917) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HG3  | 26       | 0.11          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 1        | 0.11          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 2        | 0.11          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 3        | 0.11          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 7        | 0.11          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 8        | 0.11          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 9        | 0.11          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 10       | 0.11          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 14       | 0.11          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 15       | 0.11          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 18       | 0.11          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 19       | 0.11          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 20       | 0.11          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 22       | 0.11          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 23       | 0.11          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 25       | 0.11          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 26       | 0.11          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 28       | 0.11          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 30       | 0.11          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 31       | 0.11          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 32       | 0.11          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 34       | 0.11          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 36       | 0.11          |
| (3,2894) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 37       | 0.11          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 5        | 0.11          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 9        | 0.11          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 19       | 0.11          |
| (3,2875) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 29       | 0.11          |
| (3,2848) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA   | 6        | 0.11          |
| (3,2848) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA   | 9        | 0.11          |
| (3,2848) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA   | 22       | 0.11          |
| (3,2848) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA   | 24       | 0.11          |
| (3,2848) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA   | 25       | 0.11          |
| (3,2848) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA   | 31       | 0.11          |
| (3,2848) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA   | 32       | 0.11          |
| (3,2848) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA   | 33       | 0.11          |
| (3,2848) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA   | 36       | 0.11          |
| (3,2848) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA   | 37       | 0.11          |
| (3,2848) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA   | 38       | 0.11          |
| (3,2848) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA   | 40       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2809) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HB2  | 7        | 0.11          |
| (3,2809) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HB2  | 31       | 0.11          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 1        | 0.11          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 3        | 0.11          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 8        | 0.11          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 21       | 0.11          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 25       | 0.11          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 28       | 0.11          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 31       | 0.11          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 32       | 0.11          |
| (3,2792) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 38       | 0.11          |
| (3,2761) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 13       | 0.11          |
| (3,2761) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 29       | 0.11          |
| (3,2748) | 1:86:A:GLU:HG3  | 1:87:A:PRO:HA   | 3        | 0.11          |
| (3,2720) | 1:48:A:GLU:HA   | 1:41:A:THR:HG21 | 12       | 0.11          |
| (3,2720) | 1:48:A:GLU:HA   | 1:41:A:THR:HG22 | 12       | 0.11          |
| (3,2720) | 1:48:A:GLU:HA   | 1:41:A:THR:HG23 | 12       | 0.11          |
| (3,2719) | 1:48:A:GLU:HA   | 1:49:A:LEU:HG   | 26       | 0.11          |
| (3,2717) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 9        | 0.11          |
| (3,2717) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 11       | 0.11          |
| (3,2717) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 14       | 0.11          |
| (3,2717) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 20       | 0.11          |
| (3,2717) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 29       | 0.11          |
| (3,2717) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 35       | 0.11          |
| (3,2717) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 39       | 0.11          |
| (3,2703) | 1:23:A:GLU:HA   | 1:24:A:HIS:HA   | 2        | 0.11          |
| (3,2703) | 1:23:A:GLU:HA   | 1:24:A:HIS:HA   | 5        | 0.11          |
| (3,2703) | 1:23:A:GLU:HA   | 1:24:A:HIS:HA   | 8        | 0.11          |
| (3,2703) | 1:23:A:GLU:HA   | 1:24:A:HIS:HA   | 12       | 0.11          |
| (3,2703) | 1:23:A:GLU:HA   | 1:24:A:HIS:HA   | 13       | 0.11          |
| (3,2703) | 1:23:A:GLU:HA   | 1:24:A:HIS:HA   | 19       | 0.11          |
| (3,2703) | 1:23:A:GLU:HA   | 1:24:A:HIS:HA   | 20       | 0.11          |
| (3,2703) | 1:23:A:GLU:HA   | 1:24:A:HIS:HA   | 23       | 0.11          |
| (3,2703) | 1:23:A:GLU:HA   | 1:24:A:HIS:HA   | 24       | 0.11          |
| (3,2703) | 1:23:A:GLU:HA   | 1:24:A:HIS:HA   | 28       | 0.11          |
| (3,2703) | 1:23:A:GLU:HA   | 1:24:A:HIS:HA   | 31       | 0.11          |
| (3,2703) | 1:23:A:GLU:HA   | 1:24:A:HIS:HA   | 36       | 0.11          |
| (3,2703) | 1:23:A:GLU:HA   | 1:24:A:HIS:HA   | 38       | 0.11          |
| (3,2703) | 1:23:A:GLU:HA   | 1:24:A:HIS:HA   | 39       | 0.11          |
| (3,2690) | 1:8:A:GLU:HB3   | 1:8:A:GLU:HG2   | 7        | 0.11          |
| (3,2683) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HG2  | 5        | 0.11          |
| (3,2683) | 1:53:A:GLN:HB2  | 1:53:A:GLN:HG2  | 8        | 0.11          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 9        | 0.11          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 10       | 0.11          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 15       | 0.11          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 16       | 0.11          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 21       | 0.11          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 23       | 0.11          |
| (3,2683) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 24       | 0.11          |
| (3,2679) | 1:25:A:GLN:HG3 | 1:26:A:SER:H    | 9        | 0.11          |
| (3,2679) | 1:25:A:GLN:HG3 | 1:26:A:SER:H    | 17       | 0.11          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 13       | 0.11          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 13       | 0.11          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 13       | 0.11          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 18       | 0.11          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 18       | 0.11          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 18       | 0.11          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 35       | 0.11          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 35       | 0.11          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 35       | 0.11          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 38       | 0.11          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 38       | 0.11          |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 38       | 0.11          |
| (3,2653) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 13       | 0.11          |
| (3,2653) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 14       | 0.11          |
| (3,2653) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 16       | 0.11          |
| (3,2653) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 20       | 0.11          |
| (3,2653) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 21       | 0.11          |
| (3,2653) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 30       | 0.11          |
| (3,2653) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 33       | 0.11          |
| (3,2650) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3   | 25       | 0.11          |
| (3,2650) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3   | 26       | 0.11          |
| (3,2650) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3   | 29       | 0.11          |
| (3,2650) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3   | 30       | 0.11          |
| (3,2650) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3   | 31       | 0.11          |
| (3,2650) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3   | 37       | 0.11          |
| (3,2650) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3   | 38       | 0.11          |
| (3,2650) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3   | 39       | 0.11          |
| (3,2613) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 20       | 0.11          |
| (3,2613) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 21       | 0.11          |
| (3,2613) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 23       | 0.11          |
| (3,2613) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 24       | 0.11          |
| (3,2613) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 26       | 0.11          |
| (3,2613) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 30       | 0.11          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,2613) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 33       | 0.11          |
| (3,2612) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 20       | 0.11          |
| (3,2612) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 21       | 0.11          |
| (3,2612) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 23       | 0.11          |
| (3,2612) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 24       | 0.11          |
| (3,2612) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 26       | 0.11          |
| (3,2612) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 30       | 0.11          |
| (3,2612) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 33       | 0.11          |
| (3,2554) | 1:92:A:ARG:HA  | 1:83:A:ALA:H    | 31       | 0.11          |
| (3,2529) | 1:87:A:PRO:HB3 | 1:86:A:GLU:HA   | 28       | 0.11          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2   | 21       | 0.11          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2   | 22       | 0.11          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2   | 24       | 0.11          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2   | 25       | 0.11          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2   | 27       | 0.11          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2   | 29       | 0.11          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2   | 30       | 0.11          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2   | 31       | 0.11          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2   | 32       | 0.11          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2   | 34       | 0.11          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2   | 35       | 0.11          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2   | 36       | 0.11          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2   | 37       | 0.11          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2   | 38       | 0.11          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2   | 39       | 0.11          |
| (3,2501) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2   | 40       | 0.11          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA    | 26       | 0.11          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA    | 29       | 0.11          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA    | 33       | 0.11          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA    | 35       | 0.11          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA    | 36       | 0.11          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA    | 37       | 0.11          |
| (3,2494) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA    | 39       | 0.11          |
| (3,2482) | 1:9:A:PRO:HD2  | 1:8:A:GLU:HA    | 3        | 0.11          |
| (3,2434) | 1:82:A:ILE:HB  | 1:41:A:THR:H    | 6        | 0.11          |
| (3,2434) | 1:82:A:ILE:HB  | 1:41:A:THR:H    | 7        | 0.11          |
| (3,2434) | 1:82:A:ILE:HB  | 1:41:A:THR:H    | 30       | 0.11          |
| (3,2434) | 1:82:A:ILE:HB  | 1:41:A:THR:H    | 31       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD11 | 1        | 0.11          |
| (3,2427) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD12 | 1        | 0.11          |
| (3,2427) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD13 | 1        | 0.11          |
| (3,2427) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD11 | 3        | 0.11          |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 3        | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 3        | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 4        | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 4        | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 4        | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 5        | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 5        | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 5        | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 6        | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 6        | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 6        | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 7        | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 7        | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 7        | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 8        | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 8        | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 8        | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 9        | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 9        | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 9        | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 10       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 10       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 10       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 12       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 12       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 12       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 13       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 13       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 13       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 14       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 14       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 14       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 15       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 15       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 15       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 16       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 16       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 16       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 17       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 17       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 17       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 18       | 0.11          |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 18       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 18       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 19       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 19       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 19       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 20       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 20       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 20       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 21       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 21       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 21       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 22       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 22       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 22       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 23       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 23       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 23       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 25       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 25       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 25       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 26       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 26       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 26       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 27       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 27       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 27       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 28       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 28       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 28       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 29       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 29       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 29       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 30       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 30       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 30       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 31       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 31       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 31       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 32       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 32       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 32       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 33       | 0.11          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,2427) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD12 | 33       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD13 | 33       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD11 | 34       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD12 | 34       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD13 | 34       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD11 | 35       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD12 | 35       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD13 | 35       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD11 | 37       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD12 | 37       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD13 | 37       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD11 | 39       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD12 | 39       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD13 | 39       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD11 | 40       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD12 | 40       | 0.11          |
| (3,2427) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD13 | 40       | 0.11          |
| (3,2419) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 3        | 0.11          |
| (3,2419) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 4        | 0.11          |
| (3,2419) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 7        | 0.11          |
| (3,2419) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 37       | 0.11          |
| (3,2419) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 38       | 0.11          |
| (3,2419) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 39       | 0.11          |
| (3,2406) | 1:66:A:MET:HE1 | 1:42:A:TRP:H    | 39       | 0.11          |
| (3,2406) | 1:66:A:MET:HE2 | 1:42:A:TRP:H    | 39       | 0.11          |
| (3,2406) | 1:66:A:MET:HE3 | 1:42:A:TRP:H    | 39       | 0.11          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ   | 6        | 0.11          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ   | 6        | 0.11          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ   | 6        | 0.11          |
| (3,2405) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ   | 33       | 0.11          |
| (3,2405) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ   | 33       | 0.11          |
| (3,2405) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ   | 33       | 0.11          |
| (3,2334) | 1:26:A:SER:HA  | 1:68:A:ILE:HG21 | 11       | 0.11          |
| (3,2334) | 1:26:A:SER:HA  | 1:68:A:ILE:HG22 | 11       | 0.11          |
| (3,2334) | 1:26:A:SER:HA  | 1:68:A:ILE:HG23 | 11       | 0.11          |
| (3,2334) | 1:26:A:SER:HA  | 1:68:A:ILE:HG21 | 23       | 0.11          |
| (3,2334) | 1:26:A:SER:HA  | 1:68:A:ILE:HG22 | 23       | 0.11          |
| (3,2334) | 1:26:A:SER:HA  | 1:68:A:ILE:HG23 | 23       | 0.11          |
| (3,2334) | 1:26:A:SER:HA  | 1:68:A:ILE:HG21 | 30       | 0.11          |
| (3,2334) | 1:26:A:SER:HA  | 1:68:A:ILE:HG22 | 30       | 0.11          |
| (3,2334) | 1:26:A:SER:HA  | 1:68:A:ILE:HG23 | 30       | 0.11          |
| (3,2268) | 1:96:A:GLU:HB3 | 1:78:A:VAL:HG21 | 26       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG22 | 26       | 0.11          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG23 | 26       | 0.11          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG21 | 39       | 0.11          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG22 | 39       | 0.11          |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG23 | 39       | 0.11          |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD11 | 24       | 0.11          |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD12 | 24       | 0.11          |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD13 | 24       | 0.11          |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD11 | 32       | 0.11          |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD12 | 32       | 0.11          |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD13 | 32       | 0.11          |
| (3,2148) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 11       | 0.11          |
| (3,2148) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 25       | 0.11          |
| (3,2102) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HA   | 6        | 0.11          |
| (3,2102) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HA   | 6        | 0.11          |
| (3,2102) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HA   | 6        | 0.11          |
| (3,2102) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HA   | 20       | 0.11          |
| (3,2102) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HA   | 20       | 0.11          |
| (3,2102) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HA   | 20       | 0.11          |
| (3,2102) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HA   | 33       | 0.11          |
| (3,2102) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HA   | 33       | 0.11          |
| (3,2102) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HA   | 33       | 0.11          |
| (3,2102) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HA   | 34       | 0.11          |
| (3,2102) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HA   | 34       | 0.11          |
| (3,2102) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HA   | 34       | 0.11          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 7        | 0.11          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 7        | 0.11          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 7        | 0.11          |
| (3,2099) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 19       | 0.11          |
| (3,2099) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 19       | 0.11          |
| (3,2099) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 19       | 0.11          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1  | 1        | 0.11          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2  | 1        | 0.11          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1  | 1        | 0.11          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2  | 1        | 0.11          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1  | 1        | 0.11          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2  | 1        | 0.11          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1  | 16       | 0.11          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2  | 16       | 0.11          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1  | 16       | 0.11          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2  | 16       | 0.11          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1  | 16       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2  | 16       | 0.11          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1  | 17       | 0.11          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2  | 17       | 0.11          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1  | 17       | 0.11          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2  | 17       | 0.11          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1  | 17       | 0.11          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2  | 17       | 0.11          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1  | 18       | 0.11          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2  | 18       | 0.11          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1  | 18       | 0.11          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2  | 18       | 0.11          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1  | 18       | 0.11          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2  | 18       | 0.11          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1  | 23       | 0.11          |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2  | 23       | 0.11          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1  | 23       | 0.11          |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2  | 23       | 0.11          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1  | 23       | 0.11          |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2  | 23       | 0.11          |
| (3,2075) | 1:97:A:LEU:HB2  | 1:19:A:ILE:HB   | 17       | 0.11          |
| (3,2075) | 1:97:A:LEU:HB2  | 1:19:A:ILE:HB   | 29       | 0.11          |
| (3,2074) | 1:94:A:THR:HG21 | 1:80:A:SER:HB3  | 28       | 0.11          |
| (3,2074) | 1:94:A:THR:HG22 | 1:80:A:SER:HB3  | 28       | 0.11          |
| (3,2074) | 1:94:A:THR:HG23 | 1:80:A:SER:HB3  | 28       | 0.11          |
| (3,2059) | 1:78:A:VAL:HG11 | 1:96:A:GLU:HG2  | 11       | 0.11          |
| (3,2059) | 1:78:A:VAL:HG12 | 1:96:A:GLU:HG2  | 11       | 0.11          |
| (3,2059) | 1:78:A:VAL:HG13 | 1:96:A:GLU:HG2  | 11       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD21 | 27       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD22 | 27       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD23 | 27       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD21 | 27       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD22 | 27       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD23 | 27       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD21 | 27       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD22 | 27       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD23 | 27       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD21 | 29       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD22 | 29       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD23 | 29       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD21 | 29       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD22 | 29       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD23 | 29       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD21 | 29       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD22 | 29       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD23 | 29       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD21 | 36       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD22 | 36       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD23 | 36       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD21 | 36       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD22 | 36       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD23 | 36       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD21 | 36       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD22 | 36       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD23 | 36       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD21 | 39       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD22 | 39       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD23 | 39       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD21 | 39       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD22 | 39       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD23 | 39       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD21 | 39       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD22 | 39       | 0.11          |
| (3,2058) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD23 | 39       | 0.11          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1  | 7        | 0.11          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2  | 7        | 0.11          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1  | 7        | 0.11          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2  | 7        | 0.11          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1  | 7        | 0.11          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2  | 7        | 0.11          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1  | 28       | 0.11          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2  | 28       | 0.11          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1  | 28       | 0.11          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2  | 28       | 0.11          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1  | 28       | 0.11          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2  | 28       | 0.11          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1  | 39       | 0.11          |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2  | 39       | 0.11          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1  | 39       | 0.11          |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2  | 39       | 0.11          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1  | 39       | 0.11          |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2  | 39       | 0.11          |
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3  | 4        | 0.11          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3  | 4        | 0.11          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3  | 4        | 0.11          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 6        | 0.11          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 6        | 0.11          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 6        | 0.11          |
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 10       | 0.11          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 10       | 0.11          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 10       | 0.11          |
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 24       | 0.11          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 24       | 0.11          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 24       | 0.11          |
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 33       | 0.11          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 33       | 0.11          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 33       | 0.11          |
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 37       | 0.11          |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 37       | 0.11          |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 37       | 0.11          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 23       | 0.11          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 23       | 0.11          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 23       | 0.11          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 23       | 0.11          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 23       | 0.11          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 23       | 0.11          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 28       | 0.11          |
| (3,2024) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 28       | 0.11          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 28       | 0.11          |
| (3,2024) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 28       | 0.11          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 28       | 0.11          |
| (3,2024) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 28       | 0.11          |
| (3,2019) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD1 | 1        | 0.11          |
| (3,2019) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD2 | 1        | 0.11          |
| (3,2019) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD1 | 6        | 0.11          |
| (3,2019) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD2 | 6        | 0.11          |
| (3,2019) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD1 | 12       | 0.11          |
| (3,2019) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD2 | 12       | 0.11          |
| (3,2019) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD1 | 27       | 0.11          |
| (3,2019) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD2 | 27       | 0.11          |
| (3,2019) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD1 | 39       | 0.11          |
| (3,2019) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD2 | 39       | 0.11          |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1 | 2        | 0.11          |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2 | 2        | 0.11          |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3 | 2        | 0.11          |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1 | 2        | 0.11          |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2 | 2        | 0.11          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3 | 2        | 0.11          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1 | 2        | 0.11          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2 | 2        | 0.11          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3 | 2        | 0.11          |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1 | 13       | 0.11          |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2 | 13       | 0.11          |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3 | 13       | 0.11          |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1 | 13       | 0.11          |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2 | 13       | 0.11          |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3 | 13       | 0.11          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1 | 13       | 0.11          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2 | 13       | 0.11          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3 | 13       | 0.11          |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1 | 14       | 0.11          |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2 | 14       | 0.11          |
| (3,2013) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3 | 14       | 0.11          |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1 | 14       | 0.11          |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2 | 14       | 0.11          |
| (3,2013) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3 | 14       | 0.11          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1 | 14       | 0.11          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2 | 14       | 0.11          |
| (3,2013) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3 | 14       | 0.11          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 12       | 0.11          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 29       | 0.11          |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 38       | 0.11          |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2 | 19       | 0.11          |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2 | 19       | 0.11          |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2 | 19       | 0.11          |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2 | 23       | 0.11          |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2 | 23       | 0.11          |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2 | 23       | 0.11          |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2 | 24       | 0.11          |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2 | 24       | 0.11          |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2 | 24       | 0.11          |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2 | 33       | 0.11          |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2 | 33       | 0.11          |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2 | 33       | 0.11          |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2 | 38       | 0.11          |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2 | 38       | 0.11          |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2 | 38       | 0.11          |
| (3,1997) | 1:21:A:VAL:HG11 | 1:25:A:GLN:HG3 | 8        | 0.11          |
| (3,1997) | 1:21:A:VAL:HG12 | 1:25:A:GLN:HG3 | 8        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1997) | 1:21:A:VAL:HG13 | 1:25:A:GLN:HG3  | 8        | 0.11          |
| (3,1997) | 1:21:A:VAL:HG11 | 1:25:A:GLN:HG3  | 16       | 0.11          |
| (3,1997) | 1:21:A:VAL:HG12 | 1:25:A:GLN:HG3  | 16       | 0.11          |
| (3,1997) | 1:21:A:VAL:HG13 | 1:25:A:GLN:HG3  | 16       | 0.11          |
| (3,1997) | 1:21:A:VAL:HG11 | 1:25:A:GLN:HG3  | 33       | 0.11          |
| (3,1997) | 1:21:A:VAL:HG12 | 1:25:A:GLN:HG3  | 33       | 0.11          |
| (3,1997) | 1:21:A:VAL:HG13 | 1:25:A:GLN:HG3  | 33       | 0.11          |
| (3,1997) | 1:21:A:VAL:HG11 | 1:25:A:GLN:HG3  | 38       | 0.11          |
| (3,1997) | 1:21:A:VAL:HG12 | 1:25:A:GLN:HG3  | 38       | 0.11          |
| (3,1997) | 1:21:A:VAL:HG13 | 1:25:A:GLN:HG3  | 38       | 0.11          |
| (3,1993) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 10       | 0.11          |
| (3,1993) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 10       | 0.11          |
| (3,1993) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 10       | 0.11          |
| (3,1993) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 13       | 0.11          |
| (3,1993) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 13       | 0.11          |
| (3,1993) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 13       | 0.11          |
| (3,1993) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 31       | 0.11          |
| (3,1993) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 31       | 0.11          |
| (3,1993) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 31       | 0.11          |
| (3,1993) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 32       | 0.11          |
| (3,1993) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 32       | 0.11          |
| (3,1993) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 32       | 0.11          |
| (3,1993) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 37       | 0.11          |
| (3,1993) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 37       | 0.11          |
| (3,1993) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 37       | 0.11          |
| (3,1993) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 39       | 0.11          |
| (3,1993) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 39       | 0.11          |
| (3,1993) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 39       | 0.11          |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 18       | 0.11          |
| (3,1959) | 1:72:A:THR:HG21 | 1:74:A:ASP:HB3  | 7        | 0.11          |
| (3,1959) | 1:72:A:THR:HG22 | 1:74:A:ASP:HB3  | 7        | 0.11          |
| (3,1959) | 1:72:A:THR:HG23 | 1:74:A:ASP:HB3  | 7        | 0.11          |
| (3,1959) | 1:72:A:THR:HG21 | 1:74:A:ASP:HB3  | 31       | 0.11          |
| (3,1959) | 1:72:A:THR:HG22 | 1:74:A:ASP:HB3  | 31       | 0.11          |
| (3,1959) | 1:72:A:THR:HG23 | 1:74:A:ASP:HB3  | 31       | 0.11          |
| (3,1955) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB1  | 9        | 0.11          |
| (3,1955) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB2  | 9        | 0.11          |
| (3,1955) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB3  | 9        | 0.11          |
| (3,1955) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB1  | 9        | 0.11          |
| (3,1955) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB2  | 9        | 0.11          |
| (3,1955) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB3  | 9        | 0.11          |
| (3,1955) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB1  | 9        | 0.11          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1955) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB2 | 9        | 0.11          |
| (3,1955) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB3 | 9        | 0.11          |
| (3,1955) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB1 | 17       | 0.11          |
| (3,1955) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB2 | 17       | 0.11          |
| (3,1955) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB3 | 17       | 0.11          |
| (3,1955) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB1 | 17       | 0.11          |
| (3,1955) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB2 | 17       | 0.11          |
| (3,1955) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB3 | 17       | 0.11          |
| (3,1955) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB1 | 17       | 0.11          |
| (3,1955) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB2 | 17       | 0.11          |
| (3,1955) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB3 | 17       | 0.11          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 1        | 0.11          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 1        | 0.11          |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 1        | 0.11          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 2        | 0.11          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 2        | 0.11          |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 2        | 0.11          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 5        | 0.11          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 5        | 0.11          |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 5        | 0.11          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 9        | 0.11          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 9        | 0.11          |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 9        | 0.11          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 15       | 0.11          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 15       | 0.11          |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 15       | 0.11          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 17       | 0.11          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 17       | 0.11          |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 17       | 0.11          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 26       | 0.11          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 26       | 0.11          |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 26       | 0.11          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 28       | 0.11          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 28       | 0.11          |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 28       | 0.11          |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 29       | 0.11          |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 29       | 0.11          |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 29       | 0.11          |
| (3,1910) | 1:68:A:ILE:HG21 | 1:54:A:LYS:HD2 | 28       | 0.11          |
| (3,1910) | 1:68:A:ILE:HG22 | 1:54:A:LYS:HD2 | 28       | 0.11          |
| (3,1910) | 1:68:A:ILE:HG23 | 1:54:A:LYS:HD2 | 28       | 0.11          |
| (3,1906) | 1:66:A:MET:HE1  | 1:79:A:TYR:HA  | 16       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1906) | 1:66:A:MET:HE2  | 1:79:A:TYR:HA   | 16       | 0.11          |
| (3,1906) | 1:66:A:MET:HE3  | 1:79:A:TYR:HA   | 16       | 0.11          |
| (3,1906) | 1:66:A:MET:HE1  | 1:79:A:TYR:HA   | 21       | 0.11          |
| (3,1906) | 1:66:A:MET:HE2  | 1:79:A:TYR:HA   | 21       | 0.11          |
| (3,1906) | 1:66:A:MET:HE3  | 1:79:A:TYR:HA   | 21       | 0.11          |
| (3,1904) | 1:49:A:LEU:HD21 | 1:44:A:LYS:HG2  | 2        | 0.11          |
| (3,1904) | 1:49:A:LEU:HD22 | 1:44:A:LYS:HG2  | 2        | 0.11          |
| (3,1904) | 1:49:A:LEU:HD23 | 1:44:A:LYS:HG2  | 2        | 0.11          |
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA   | 7        | 0.11          |
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA   | 7        | 0.11          |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA   | 7        | 0.11          |
| (3,1902) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA   | 11       | 0.11          |
| (3,1902) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA   | 11       | 0.11          |
| (3,1902) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA   | 11       | 0.11          |
| (3,1899) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3  | 2        | 0.11          |
| (3,1899) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3  | 2        | 0.11          |
| (3,1899) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3  | 2        | 0.11          |
| (3,1899) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3  | 12       | 0.11          |
| (3,1899) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3  | 12       | 0.11          |
| (3,1899) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3  | 12       | 0.11          |
| (3,1864) | 1:7:A:ALA:HB1   | 1:88:A:ARG:HA   | 1        | 0.11          |
| (3,1864) | 1:7:A:ALA:HB2   | 1:88:A:ARG:HA   | 1        | 0.11          |
| (3,1864) | 1:7:A:ALA:HB3   | 1:88:A:ARG:HA   | 1        | 0.11          |
| (3,1864) | 1:7:A:ALA:HB1   | 1:88:A:ARG:HA   | 36       | 0.11          |
| (3,1864) | 1:7:A:ALA:HB2   | 1:88:A:ARG:HA   | 36       | 0.11          |
| (3,1864) | 1:7:A:ALA:HB3   | 1:88:A:ARG:HA   | 36       | 0.11          |
| (3,1864) | 1:7:A:ALA:HB1   | 1:88:A:ARG:HA   | 39       | 0.11          |
| (3,1864) | 1:7:A:ALA:HB2   | 1:88:A:ARG:HA   | 39       | 0.11          |
| (3,1864) | 1:7:A:ALA:HB3   | 1:88:A:ARG:HA   | 39       | 0.11          |
| (3,1721) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG11 | 22       | 0.11          |
| (3,1721) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG12 | 22       | 0.11          |
| (3,1721) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG13 | 22       | 0.11          |
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG11 | 22       | 0.11          |
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG12 | 22       | 0.11          |
| (3,1721) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 22       | 0.11          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 22       | 0.11          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 22       | 0.11          |
| (3,1721) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 22       | 0.11          |
| (3,1712) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 6        | 0.11          |
| (3,1712) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 6        | 0.11          |
| (3,1712) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 6        | 0.11          |
| (3,1712) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 7        | 0.11          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (3,1712) | 1:49:A:LEU:HD22  | 1:49:A:LEU:H    | 7        | 0.11          |
| (3,1712) | 1:49:A:LEU:HD23  | 1:49:A:LEU:H    | 7        | 0.11          |
| (3,1712) | 1:49:A:LEU:HD21  | 1:49:A:LEU:H    | 8        | 0.11          |
| (3,1712) | 1:49:A:LEU:HD22  | 1:49:A:LEU:H    | 8        | 0.11          |
| (3,1712) | 1:49:A:LEU:HD23  | 1:49:A:LEU:H    | 8        | 0.11          |
| (3,1712) | 1:49:A:LEU:HD21  | 1:49:A:LEU:H    | 21       | 0.11          |
| (3,1712) | 1:49:A:LEU:HD22  | 1:49:A:LEU:H    | 21       | 0.11          |
| (3,1712) | 1:49:A:LEU:HD23  | 1:49:A:LEU:H    | 21       | 0.11          |
| (3,1712) | 1:49:A:LEU:HD21  | 1:49:A:LEU:H    | 23       | 0.11          |
| (3,1712) | 1:49:A:LEU:HD22  | 1:49:A:LEU:H    | 23       | 0.11          |
| (3,1712) | 1:49:A:LEU:HD23  | 1:49:A:LEU:H    | 23       | 0.11          |
| (3,1712) | 1:49:A:LEU:HD21  | 1:49:A:LEU:H    | 30       | 0.11          |
| (3,1712) | 1:49:A:LEU:HD22  | 1:49:A:LEU:H    | 30       | 0.11          |
| (3,1712) | 1:49:A:LEU:HD23  | 1:49:A:LEU:H    | 30       | 0.11          |
| (3,1712) | 1:49:A:LEU:HD21  | 1:49:A:LEU:H    | 32       | 0.11          |
| (3,1712) | 1:49:A:LEU:HD22  | 1:49:A:LEU:H    | 32       | 0.11          |
| (3,1712) | 1:49:A:LEU:HD23  | 1:49:A:LEU:H    | 32       | 0.11          |
| (3,1712) | 1:49:A:LEU:HD21  | 1:49:A:LEU:H    | 33       | 0.11          |
| (3,1712) | 1:49:A:LEU:HD22  | 1:49:A:LEU:H    | 33       | 0.11          |
| (3,1712) | 1:49:A:LEU:HD23  | 1:49:A:LEU:H    | 33       | 0.11          |
| (3,1712) | 1:49:A:LEU:HD21  | 1:49:A:LEU:H    | 34       | 0.11          |
| (3,1712) | 1:49:A:LEU:HD22  | 1:49:A:LEU:H    | 34       | 0.11          |
| (3,1712) | 1:49:A:LEU:HD23  | 1:49:A:LEU:H    | 34       | 0.11          |
| (3,1712) | 1:49:A:LEU:HD21  | 1:49:A:LEU:H    | 35       | 0.11          |
| (3,1712) | 1:49:A:LEU:HD22  | 1:49:A:LEU:H    | 35       | 0.11          |
| (3,1712) | 1:49:A:LEU:HD23  | 1:49:A:LEU:H    | 35       | 0.11          |
| (3,1712) | 1:49:A:LEU:HD21  | 1:49:A:LEU:H    | 39       | 0.11          |
| (3,1712) | 1:49:A:LEU:HD22  | 1:49:A:LEU:H    | 39       | 0.11          |
| (3,1712) | 1:49:A:LEU:HD23  | 1:49:A:LEU:H    | 39       | 0.11          |
| (3,1712) | 1:49:A:LEU:HD21  | 1:49:A:LEU:H    | 40       | 0.11          |
| (3,1712) | 1:49:A:LEU:HD22  | 1:49:A:LEU:H    | 40       | 0.11          |
| (3,1712) | 1:49:A:LEU:HD23  | 1:49:A:LEU:H    | 40       | 0.11          |
| (3,1710) | 1:49:A:LEU:HD21  | 1:50:A:THR:H    | 35       | 0.11          |
| (3,1710) | 1:49:A:LEU:HD22  | 1:50:A:THR:H    | 35       | 0.11          |
| (3,1710) | 1:49:A:LEU:HD23  | 1:50:A:THR:H    | 35       | 0.11          |
| (3,1700) | 1:101:A:LEU:HD21 | 1:101:A:LEU:HB3 | 31       | 0.11          |
| (3,1700) | 1:101:A:LEU:HD22 | 1:101:A:LEU:HB3 | 31       | 0.11          |
| (3,1700) | 1:101:A:LEU:HD23 | 1:101:A:LEU:HB3 | 31       | 0.11          |
| (3,1689) | 1:97:A:LEU:HD11  | 1:71:A:VAL:HG21 | 6        | 0.11          |
| (3,1689) | 1:97:A:LEU:HD11  | 1:71:A:VAL:HG22 | 6        | 0.11          |
| (3,1689) | 1:97:A:LEU:HD11  | 1:71:A:VAL:HG23 | 6        | 0.11          |
| (3,1689) | 1:97:A:LEU:HD12  | 1:71:A:VAL:HG21 | 6        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 6        | 0.11          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 6        | 0.11          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 6        | 0.11          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 6        | 0.11          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 6        | 0.11          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 7        | 0.11          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 7        | 0.11          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 7        | 0.11          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 7        | 0.11          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 7        | 0.11          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 7        | 0.11          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 7        | 0.11          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 7        | 0.11          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 7        | 0.11          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG21 | 23       | 0.11          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG22 | 23       | 0.11          |
| (3,1689) | 1:97:A:LEU:HD11 | 1:71:A:VAL:HG23 | 23       | 0.11          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG21 | 23       | 0.11          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG22 | 23       | 0.11          |
| (3,1689) | 1:97:A:LEU:HD12 | 1:71:A:VAL:HG23 | 23       | 0.11          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG21 | 23       | 0.11          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG22 | 23       | 0.11          |
| (3,1689) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 23       | 0.11          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 30       | 0.11          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 30       | 0.11          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 30       | 0.11          |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 39       | 0.11          |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 39       | 0.11          |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 39       | 0.11          |
| (3,1658) | 1:40:A:VAL:HB   | 1:39:A:ILE:HA   | 2        | 0.11          |
| (3,1658) | 1:40:A:VAL:HB   | 1:39:A:ILE:HA   | 24       | 0.11          |
| (3,1658) | 1:40:A:VAL:HB   | 1:39:A:ILE:HA   | 36       | 0.11          |
| (3,1654) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 4        | 0.11          |
| (3,1654) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 4        | 0.11          |
| (3,1654) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 4        | 0.11          |
| (3,1654) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 4        | 0.11          |
| (3,1654) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 4        | 0.11          |
| (3,1654) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 4        | 0.11          |
| (3,1654) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 4        | 0.11          |
| (3,1654) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 4        | 0.11          |
| (3,1654) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 4        | 0.11          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 15       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 15       | 0.11          |
| (3,1643) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 15       | 0.11          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 15       | 0.11          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 15       | 0.11          |
| (3,1643) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 15       | 0.11          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 15       | 0.11          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 15       | 0.11          |
| (3,1643) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 15       | 0.11          |
| (3,1628) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2  | 17       | 0.11          |
| (3,1628) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2  | 17       | 0.11          |
| (3,1628) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2  | 17       | 0.11          |
| (3,1628) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2  | 31       | 0.11          |
| (3,1628) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2  | 31       | 0.11          |
| (3,1628) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2  | 31       | 0.11          |
| (3,1627) | 1:82:A:ILE:HG21 | 1:84:A:ARG:HG2  | 20       | 0.11          |
| (3,1627) | 1:82:A:ILE:HG22 | 1:84:A:ARG:HG2  | 20       | 0.11          |
| (3,1627) | 1:82:A:ILE:HG23 | 1:84:A:ARG:HG2  | 20       | 0.11          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1  | 6        | 0.11          |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2  | 6        | 0.11          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1  | 6        | 0.11          |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2  | 6        | 0.11          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1  | 6        | 0.11          |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2  | 6        | 0.11          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 3        | 0.11          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 3        | 0.11          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 3        | 0.11          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 3        | 0.11          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 3        | 0.11          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 3        | 0.11          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 6        | 0.11          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 6        | 0.11          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 6        | 0.11          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 6        | 0.11          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 6        | 0.11          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 6        | 0.11          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 29       | 0.11          |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 29       | 0.11          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 29       | 0.11          |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 29       | 0.11          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 29       | 0.11          |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 29       | 0.11          |
| (3,1554) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA    | 21       | 0.11          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1554) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA   | 21       | 0.11          |
| (3,1554) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA   | 21       | 0.11          |
| (3,1554) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA   | 24       | 0.11          |
| (3,1554) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA   | 24       | 0.11          |
| (3,1554) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA   | 24       | 0.11          |
| (3,1554) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA   | 25       | 0.11          |
| (3,1554) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA   | 25       | 0.11          |
| (3,1554) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA   | 25       | 0.11          |
| (3,1554) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA   | 32       | 0.11          |
| (3,1554) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA   | 32       | 0.11          |
| (3,1554) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA   | 32       | 0.11          |
| (3,1554) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA   | 37       | 0.11          |
| (3,1554) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA   | 37       | 0.11          |
| (3,1554) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA   | 37       | 0.11          |
| (3,1554) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA   | 38       | 0.11          |
| (3,1554) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA   | 38       | 0.11          |
| (3,1554) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA   | 38       | 0.11          |
| (3,1552) | 1:10:A:ILE:HG21 | 1:83:A:ALA:HB1 | 3        | 0.11          |
| (3,1552) | 1:10:A:ILE:HG21 | 1:83:A:ALA:HB2 | 3        | 0.11          |
| (3,1552) | 1:10:A:ILE:HG21 | 1:83:A:ALA:HB3 | 3        | 0.11          |
| (3,1552) | 1:10:A:ILE:HG22 | 1:83:A:ALA:HB1 | 3        | 0.11          |
| (3,1552) | 1:10:A:ILE:HG22 | 1:83:A:ALA:HB2 | 3        | 0.11          |
| (3,1552) | 1:10:A:ILE:HG22 | 1:83:A:ALA:HB3 | 3        | 0.11          |
| (3,1552) | 1:10:A:ILE:HG23 | 1:83:A:ALA:HB1 | 3        | 0.11          |
| (3,1552) | 1:10:A:ILE:HG23 | 1:83:A:ALA:HB2 | 3        | 0.11          |
| (3,1552) | 1:10:A:ILE:HG23 | 1:83:A:ALA:HB3 | 3        | 0.11          |
| (3,1552) | 1:10:A:ILE:HG21 | 1:83:A:ALA:HB1 | 10       | 0.11          |
| (3,1552) | 1:10:A:ILE:HG21 | 1:83:A:ALA:HB2 | 10       | 0.11          |
| (3,1552) | 1:10:A:ILE:HG21 | 1:83:A:ALA:HB3 | 10       | 0.11          |
| (3,1552) | 1:10:A:ILE:HG22 | 1:83:A:ALA:HB1 | 10       | 0.11          |
| (3,1552) | 1:10:A:ILE:HG22 | 1:83:A:ALA:HB2 | 10       | 0.11          |
| (3,1552) | 1:10:A:ILE:HG22 | 1:83:A:ALA:HB3 | 10       | 0.11          |
| (3,1552) | 1:10:A:ILE:HG23 | 1:83:A:ALA:HB1 | 10       | 0.11          |
| (3,1552) | 1:10:A:ILE:HG23 | 1:83:A:ALA:HB2 | 10       | 0.11          |
| (3,1552) | 1:10:A:ILE:HG23 | 1:83:A:ALA:HB3 | 10       | 0.11          |
| (3,1552) | 1:10:A:ILE:HG21 | 1:83:A:ALA:HB1 | 14       | 0.11          |
| (3,1552) | 1:10:A:ILE:HG21 | 1:83:A:ALA:HB2 | 14       | 0.11          |
| (3,1552) | 1:10:A:ILE:HG21 | 1:83:A:ALA:HB3 | 14       | 0.11          |
| (3,1552) | 1:10:A:ILE:HG22 | 1:83:A:ALA:HB1 | 14       | 0.11          |
| (3,1552) | 1:10:A:ILE:HG22 | 1:83:A:ALA:HB2 | 14       | 0.11          |
| (3,1552) | 1:10:A:ILE:HG22 | 1:83:A:ALA:HB3 | 14       | 0.11          |
| (3,1552) | 1:10:A:ILE:HG23 | 1:83:A:ALA:HB1 | 14       | 0.11          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (3,1552) | 1:10:A:ILE:HG23 | 1:83:A:ALA:HB2 | 14       | 0.11          |
| (3,1552) | 1:10:A:ILE:HG23 | 1:83:A:ALA:HB3 | 14       | 0.11          |
| (3,1522) | 1:66:A:MET:HE1  | 1:66:A:MET:HA  | 6        | 0.11          |
| (3,1522) | 1:66:A:MET:HE2  | 1:66:A:MET:HA  | 6        | 0.11          |
| (3,1522) | 1:66:A:MET:HE3  | 1:66:A:MET:HA  | 6        | 0.11          |
| (3,1517) | 1:66:A:MET:HE1  | 1:29:A:PHE:H   | 9        | 0.11          |
| (3,1517) | 1:66:A:MET:HE2  | 1:29:A:PHE:H   | 9        | 0.11          |
| (3,1517) | 1:66:A:MET:HE3  | 1:29:A:PHE:H   | 9        | 0.11          |
| (3,1517) | 1:66:A:MET:HE1  | 1:29:A:PHE:H   | 14       | 0.11          |
| (3,1517) | 1:66:A:MET:HE2  | 1:29:A:PHE:H   | 14       | 0.11          |
| (3,1517) | 1:66:A:MET:HE3  | 1:29:A:PHE:H   | 14       | 0.11          |
| (3,1517) | 1:66:A:MET:HE1  | 1:29:A:PHE:H   | 22       | 0.11          |
| (3,1517) | 1:66:A:MET:HE2  | 1:29:A:PHE:H   | 22       | 0.11          |
| (3,1517) | 1:66:A:MET:HE3  | 1:29:A:PHE:H   | 22       | 0.11          |
| (3,1517) | 1:66:A:MET:HE1  | 1:29:A:PHE:H   | 25       | 0.11          |
| (3,1517) | 1:66:A:MET:HE2  | 1:29:A:PHE:H   | 25       | 0.11          |
| (3,1517) | 1:66:A:MET:HE3  | 1:29:A:PHE:H   | 25       | 0.11          |
| (3,1517) | 1:66:A:MET:HE1  | 1:29:A:PHE:H   | 30       | 0.11          |
| (3,1517) | 1:66:A:MET:HE2  | 1:29:A:PHE:H   | 30       | 0.11          |
| (3,1517) | 1:66:A:MET:HE3  | 1:29:A:PHE:H   | 30       | 0.11          |
| (3,1514) | 1:66:A:MET:HE1  | 1:42:A:TRP:HE1 | 2        | 0.11          |
| (3,1514) | 1:66:A:MET:HE2  | 1:42:A:TRP:HE1 | 2        | 0.11          |
| (3,1514) | 1:66:A:MET:HE3  | 1:42:A:TRP:HE1 | 2        | 0.11          |
| (3,1514) | 1:66:A:MET:HE1  | 1:42:A:TRP:HE1 | 4        | 0.11          |
| (3,1514) | 1:66:A:MET:HE2  | 1:42:A:TRP:HE1 | 4        | 0.11          |
| (3,1514) | 1:66:A:MET:HE3  | 1:42:A:TRP:HE1 | 4        | 0.11          |
| (3,1514) | 1:66:A:MET:HE1  | 1:42:A:TRP:HE1 | 14       | 0.11          |
| (3,1514) | 1:66:A:MET:HE2  | 1:42:A:TRP:HE1 | 14       | 0.11          |
| (3,1514) | 1:66:A:MET:HE3  | 1:42:A:TRP:HE1 | 14       | 0.11          |
| (3,1514) | 1:66:A:MET:HE1  | 1:42:A:TRP:HE1 | 23       | 0.11          |
| (3,1514) | 1:66:A:MET:HE2  | 1:42:A:TRP:HE1 | 23       | 0.11          |
| (3,1514) | 1:66:A:MET:HE3  | 1:42:A:TRP:HE1 | 23       | 0.11          |
| (3,1514) | 1:66:A:MET:HE1  | 1:42:A:TRP:HE1 | 24       | 0.11          |
| (3,1514) | 1:66:A:MET:HE2  | 1:42:A:TRP:HE1 | 24       | 0.11          |
| (3,1514) | 1:66:A:MET:HE3  | 1:42:A:TRP:HE1 | 24       | 0.11          |
| (3,1514) | 1:66:A:MET:HE1  | 1:42:A:TRP:HE1 | 32       | 0.11          |
| (3,1514) | 1:66:A:MET:HE2  | 1:42:A:TRP:HE1 | 32       | 0.11          |
| (3,1514) | 1:66:A:MET:HE3  | 1:42:A:TRP:HE1 | 32       | 0.11          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE1 | 39       | 0.11          |
| (3,1513) | 1:66:A:MET:HE1  | 1:79:A:TYR:HE2 | 39       | 0.11          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE1 | 39       | 0.11          |
| (3,1513) | 1:66:A:MET:HE2  | 1:79:A:TYR:HE2 | 39       | 0.11          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 39       | 0.11          |
| (3,1513) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 39       | 0.11          |
| (3,1511) | 1:66:A:MET:HE1 | 1:42:A:TRP:HB2 | 3        | 0.11          |
| (3,1511) | 1:66:A:MET:HE2 | 1:42:A:TRP:HB2 | 3        | 0.11          |
| (3,1511) | 1:66:A:MET:HE3 | 1:42:A:TRP:HB2 | 3        | 0.11          |
| (3,1511) | 1:66:A:MET:HE1 | 1:42:A:TRP:HB2 | 9        | 0.11          |
| (3,1511) | 1:66:A:MET:HE2 | 1:42:A:TRP:HB2 | 9        | 0.11          |
| (3,1511) | 1:66:A:MET:HE3 | 1:42:A:TRP:HB2 | 9        | 0.11          |
| (3,1511) | 1:66:A:MET:HE1 | 1:42:A:TRP:HB2 | 11       | 0.11          |
| (3,1511) | 1:66:A:MET:HE2 | 1:42:A:TRP:HB2 | 11       | 0.11          |
| (3,1511) | 1:66:A:MET:HE3 | 1:42:A:TRP:HB2 | 11       | 0.11          |
| (3,1511) | 1:66:A:MET:HE1 | 1:42:A:TRP:HB2 | 18       | 0.11          |
| (3,1511) | 1:66:A:MET:HE2 | 1:42:A:TRP:HB2 | 18       | 0.11          |
| (3,1511) | 1:66:A:MET:HE3 | 1:42:A:TRP:HB2 | 18       | 0.11          |
| (3,1511) | 1:66:A:MET:HE1 | 1:42:A:TRP:HB2 | 20       | 0.11          |
| (3,1511) | 1:66:A:MET:HE2 | 1:42:A:TRP:HB2 | 20       | 0.11          |
| (3,1511) | 1:66:A:MET:HE3 | 1:42:A:TRP:HB2 | 20       | 0.11          |
| (3,1511) | 1:66:A:MET:HE1 | 1:42:A:TRP:HB2 | 23       | 0.11          |
| (3,1511) | 1:66:A:MET:HE2 | 1:42:A:TRP:HB2 | 23       | 0.11          |
| (3,1511) | 1:66:A:MET:HE3 | 1:42:A:TRP:HB2 | 23       | 0.11          |
| (3,1511) | 1:66:A:MET:HE1 | 1:42:A:TRP:HB2 | 25       | 0.11          |
| (3,1511) | 1:66:A:MET:HE2 | 1:42:A:TRP:HB2 | 25       | 0.11          |
| (3,1511) | 1:66:A:MET:HE3 | 1:42:A:TRP:HB2 | 25       | 0.11          |
| (3,1511) | 1:66:A:MET:HE1 | 1:42:A:TRP:HB2 | 26       | 0.11          |
| (3,1511) | 1:66:A:MET:HE2 | 1:42:A:TRP:HB2 | 26       | 0.11          |
| (3,1511) | 1:66:A:MET:HE3 | 1:42:A:TRP:HB2 | 26       | 0.11          |
| (3,1511) | 1:66:A:MET:HE1 | 1:42:A:TRP:HB2 | 30       | 0.11          |
| (3,1511) | 1:66:A:MET:HE2 | 1:42:A:TRP:HB2 | 30       | 0.11          |
| (3,1511) | 1:66:A:MET:HE3 | 1:42:A:TRP:HB2 | 30       | 0.11          |
| (3,1511) | 1:66:A:MET:HE1 | 1:42:A:TRP:HB2 | 31       | 0.11          |
| (3,1511) | 1:66:A:MET:HE2 | 1:42:A:TRP:HB2 | 31       | 0.11          |
| (3,1511) | 1:66:A:MET:HE3 | 1:42:A:TRP:HB2 | 31       | 0.11          |
| (3,1507) | 1:66:A:MET:HE1 | 1:66:A:MET:HG2 | 4        | 0.11          |
| (3,1507) | 1:66:A:MET:HE2 | 1:66:A:MET:HG2 | 4        | 0.11          |
| (3,1507) | 1:66:A:MET:HE3 | 1:66:A:MET:HG2 | 4        | 0.11          |
| (3,1507) | 1:66:A:MET:HE1 | 1:66:A:MET:HG2 | 15       | 0.11          |
| (3,1507) | 1:66:A:MET:HE2 | 1:66:A:MET:HG2 | 15       | 0.11          |
| (3,1507) | 1:66:A:MET:HE3 | 1:66:A:MET:HG2 | 15       | 0.11          |
| (3,1507) | 1:66:A:MET:HE1 | 1:66:A:MET:HG2 | 16       | 0.11          |
| (3,1507) | 1:66:A:MET:HE2 | 1:66:A:MET:HG2 | 16       | 0.11          |
| (3,1507) | 1:66:A:MET:HE3 | 1:66:A:MET:HG2 | 16       | 0.11          |
| (3,1507) | 1:66:A:MET:HE1 | 1:66:A:MET:HG2 | 19       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1507) | 1:66:A:MET:HE2  | 1:66:A:MET:HG2  | 19       | 0.11          |
| (3,1507) | 1:66:A:MET:HE3  | 1:66:A:MET:HG2  | 19       | 0.11          |
| (3,1507) | 1:66:A:MET:HE1  | 1:66:A:MET:HG2  | 29       | 0.11          |
| (3,1507) | 1:66:A:MET:HE2  | 1:66:A:MET:HG2  | 29       | 0.11          |
| (3,1507) | 1:66:A:MET:HE3  | 1:66:A:MET:HG2  | 29       | 0.11          |
| (3,1507) | 1:66:A:MET:HE1  | 1:66:A:MET:HG2  | 33       | 0.11          |
| (3,1507) | 1:66:A:MET:HE2  | 1:66:A:MET:HG2  | 33       | 0.11          |
| (3,1507) | 1:66:A:MET:HE3  | 1:66:A:MET:HG2  | 33       | 0.11          |
| (3,1507) | 1:66:A:MET:HE1  | 1:66:A:MET:HG2  | 39       | 0.11          |
| (3,1507) | 1:66:A:MET:HE2  | 1:66:A:MET:HG2  | 39       | 0.11          |
| (3,1507) | 1:66:A:MET:HE3  | 1:66:A:MET:HG2  | 39       | 0.11          |
| (3,1506) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD11 | 9        | 0.11          |
| (3,1506) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD12 | 9        | 0.11          |
| (3,1506) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD13 | 9        | 0.11          |
| (3,1506) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD11 | 9        | 0.11          |
| (3,1506) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD12 | 9        | 0.11          |
| (3,1506) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD13 | 9        | 0.11          |
| (3,1506) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD11 | 9        | 0.11          |
| (3,1506) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD12 | 9        | 0.11          |
| (3,1506) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD13 | 9        | 0.11          |
| (3,1506) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD11 | 35       | 0.11          |
| (3,1506) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD12 | 35       | 0.11          |
| (3,1506) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD13 | 35       | 0.11          |
| (3,1506) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD11 | 35       | 0.11          |
| (3,1506) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD12 | 35       | 0.11          |
| (3,1506) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD13 | 35       | 0.11          |
| (3,1506) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD11 | 35       | 0.11          |
| (3,1506) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD12 | 35       | 0.11          |
| (3,1506) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD13 | 35       | 0.11          |
| (3,1498) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 12       | 0.11          |
| (3,1498) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 12       | 0.11          |
| (3,1498) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 12       | 0.11          |
| (3,1498) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 15       | 0.11          |
| (3,1498) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 15       | 0.11          |
| (3,1498) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 15       | 0.11          |
| (3,1498) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 23       | 0.11          |
| (3,1498) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 23       | 0.11          |
| (3,1498) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 23       | 0.11          |
| (3,1498) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 33       | 0.11          |
| (3,1498) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 33       | 0.11          |
| (3,1498) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 33       | 0.11          |
| (3,1498) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 39       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1498) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 39       | 0.11          |
| (3,1498) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 39       | 0.11          |
| (3,1488) | 1:81:A:VAL:HB   | 1:42:A:TRP:HE1  | 10       | 0.11          |
| (3,1488) | 1:81:A:VAL:HB   | 1:42:A:TRP:HE1  | 11       | 0.11          |
| (3,1488) | 1:81:A:VAL:HB   | 1:42:A:TRP:HE1  | 34       | 0.11          |
| (3,1440) | 1:33:A:VAL:HG21 | 1:32:A:GLU:HA   | 27       | 0.11          |
| (3,1440) | 1:33:A:VAL:HG22 | 1:32:A:GLU:HA   | 27       | 0.11          |
| (3,1440) | 1:33:A:VAL:HG23 | 1:32:A:GLU:HA   | 27       | 0.11          |
| (3,1424) | 1:21:A:VAL:HG21 | 1:19:A:ILE:HD11 | 9        | 0.11          |
| (3,1424) | 1:21:A:VAL:HG21 | 1:19:A:ILE:HD12 | 9        | 0.11          |
| (3,1424) | 1:21:A:VAL:HG21 | 1:19:A:ILE:HD13 | 9        | 0.11          |
| (3,1424) | 1:21:A:VAL:HG22 | 1:19:A:ILE:HD11 | 9        | 0.11          |
| (3,1424) | 1:21:A:VAL:HG22 | 1:19:A:ILE:HD12 | 9        | 0.11          |
| (3,1424) | 1:21:A:VAL:HG22 | 1:19:A:ILE:HD13 | 9        | 0.11          |
| (3,1424) | 1:21:A:VAL:HG23 | 1:19:A:ILE:HD11 | 9        | 0.11          |
| (3,1424) | 1:21:A:VAL:HG23 | 1:19:A:ILE:HD12 | 9        | 0.11          |
| (3,1424) | 1:21:A:VAL:HG23 | 1:19:A:ILE:HD13 | 9        | 0.11          |
| (3,1424) | 1:21:A:VAL:HG21 | 1:19:A:ILE:HD11 | 15       | 0.11          |
| (3,1424) | 1:21:A:VAL:HG21 | 1:19:A:ILE:HD12 | 15       | 0.11          |
| (3,1424) | 1:21:A:VAL:HG21 | 1:19:A:ILE:HD13 | 15       | 0.11          |
| (3,1424) | 1:21:A:VAL:HG22 | 1:19:A:ILE:HD11 | 15       | 0.11          |
| (3,1424) | 1:21:A:VAL:HG22 | 1:19:A:ILE:HD12 | 15       | 0.11          |
| (3,1424) | 1:21:A:VAL:HG22 | 1:19:A:ILE:HD13 | 15       | 0.11          |
| (3,1424) | 1:21:A:VAL:HG23 | 1:19:A:ILE:HD11 | 15       | 0.11          |
| (3,1424) | 1:21:A:VAL:HG23 | 1:19:A:ILE:HD12 | 15       | 0.11          |
| (3,1424) | 1:21:A:VAL:HG23 | 1:19:A:ILE:HD13 | 15       | 0.11          |
| (3,1422) | 1:21:A:VAL:HG11 | 1:27:A:ALA:HB1  | 9        | 0.11          |
| (3,1422) | 1:21:A:VAL:HG11 | 1:27:A:ALA:HB2  | 9        | 0.11          |
| (3,1422) | 1:21:A:VAL:HG11 | 1:27:A:ALA:HB3  | 9        | 0.11          |
| (3,1422) | 1:21:A:VAL:HG12 | 1:27:A:ALA:HB1  | 9        | 0.11          |
| (3,1422) | 1:21:A:VAL:HG12 | 1:27:A:ALA:HB2  | 9        | 0.11          |
| (3,1422) | 1:21:A:VAL:HG12 | 1:27:A:ALA:HB3  | 9        | 0.11          |
| (3,1422) | 1:21:A:VAL:HG13 | 1:27:A:ALA:HB1  | 9        | 0.11          |
| (3,1422) | 1:21:A:VAL:HG13 | 1:27:A:ALA:HB2  | 9        | 0.11          |
| (3,1422) | 1:21:A:VAL:HG13 | 1:27:A:ALA:HB3  | 9        | 0.11          |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H    | 7        | 0.11          |
| (3,1407) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H    | 7        | 0.11          |
| (3,1407) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H    | 7        | 0.11          |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H    | 9        | 0.11          |
| (3,1407) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H    | 9        | 0.11          |
| (3,1407) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H    | 9        | 0.11          |
| (3,1407) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H    | 21       | 0.11          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,1407) | 1:95:A:ALA:HB2 | 1:18:A:ASN:H   | 21       | 0.11          |
| (3,1407) | 1:95:A:ALA:HB3 | 1:18:A:ASN:H   | 21       | 0.11          |
| (3,1407) | 1:95:A:ALA:HB1 | 1:18:A:ASN:H   | 37       | 0.11          |
| (3,1407) | 1:95:A:ALA:HB2 | 1:18:A:ASN:H   | 37       | 0.11          |
| (3,1407) | 1:95:A:ALA:HB3 | 1:18:A:ASN:H   | 37       | 0.11          |
| (3,1405) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H   | 14       | 0.11          |
| (3,1405) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H   | 14       | 0.11          |
| (3,1405) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H   | 14       | 0.11          |
| (3,1405) | 1:95:A:ALA:HB1 | 1:96:A:GLU:H   | 27       | 0.11          |
| (3,1405) | 1:95:A:ALA:HB2 | 1:96:A:GLU:H   | 27       | 0.11          |
| (3,1405) | 1:95:A:ALA:HB3 | 1:96:A:GLU:H   | 27       | 0.11          |
| (3,1400) | 1:95:A:ALA:HB1 | 1:94:A:THR:HA  | 28       | 0.11          |
| (3,1400) | 1:95:A:ALA:HB2 | 1:94:A:THR:HA  | 28       | 0.11          |
| (3,1400) | 1:95:A:ALA:HB3 | 1:94:A:THR:HA  | 28       | 0.11          |
| (3,1391) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ  | 16       | 0.11          |
| (3,1391) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ  | 16       | 0.11          |
| (3,1391) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ  | 16       | 0.11          |
| (3,1391) | 1:91:A:ALA:HB1 | 1:12:A:PHE:HZ  | 26       | 0.11          |
| (3,1391) | 1:91:A:ALA:HB2 | 1:12:A:PHE:HZ  | 26       | 0.11          |
| (3,1391) | 1:91:A:ALA:HB3 | 1:12:A:PHE:HZ  | 26       | 0.11          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 5        | 0.11          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 5        | 0.11          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 5        | 0.11          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 5        | 0.11          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 5        | 0.11          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 5        | 0.11          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 5        | 0.11          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 5        | 0.11          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 5        | 0.11          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 9        | 0.11          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 9        | 0.11          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 9        | 0.11          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 9        | 0.11          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 9        | 0.11          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 9        | 0.11          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 9        | 0.11          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 9        | 0.11          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 9        | 0.11          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 14       | 0.11          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 14       | 0.11          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 14       | 0.11          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 14       | 0.11          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 14       | 0.11          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 14       | 0.11          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 14       | 0.11          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 14       | 0.11          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 14       | 0.11          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 19       | 0.11          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 19       | 0.11          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 19       | 0.11          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 19       | 0.11          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 19       | 0.11          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 19       | 0.11          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 19       | 0.11          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 19       | 0.11          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 19       | 0.11          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 22       | 0.11          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 22       | 0.11          |
| (3,1388) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 22       | 0.11          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 22       | 0.11          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 22       | 0.11          |
| (3,1388) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 22       | 0.11          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 22       | 0.11          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 22       | 0.11          |
| (3,1388) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 22       | 0.11          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 5        | 0.11          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 5        | 0.11          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 5        | 0.11          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 5        | 0.11          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 5        | 0.11          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 5        | 0.11          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 5        | 0.11          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 5        | 0.11          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 5        | 0.11          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 9        | 0.11          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 9        | 0.11          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 9        | 0.11          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 9        | 0.11          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 9        | 0.11          |
| (3,1383) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 9        | 0.11          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 9        | 0.11          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 9        | 0.11          |
| (3,1383) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 9        | 0.11          |
| (3,1383) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 14       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1383) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB2  | 14       | 0.11          |
| (3,1383) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB3  | 14       | 0.11          |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB1  | 14       | 0.11          |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB2  | 14       | 0.11          |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB3  | 14       | 0.11          |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB1  | 14       | 0.11          |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB2  | 14       | 0.11          |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB3  | 14       | 0.11          |
| (3,1383) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB1  | 19       | 0.11          |
| (3,1383) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB2  | 19       | 0.11          |
| (3,1383) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB3  | 19       | 0.11          |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB1  | 19       | 0.11          |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB2  | 19       | 0.11          |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB3  | 19       | 0.11          |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB1  | 19       | 0.11          |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB2  | 19       | 0.11          |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB3  | 19       | 0.11          |
| (3,1383) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB1  | 22       | 0.11          |
| (3,1383) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB2  | 22       | 0.11          |
| (3,1383) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB3  | 22       | 0.11          |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB1  | 22       | 0.11          |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB2  | 22       | 0.11          |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB3  | 22       | 0.11          |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB1  | 22       | 0.11          |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB2  | 22       | 0.11          |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB3  | 22       | 0.11          |
| (3,1361) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 7        | 0.11          |
| (3,1361) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 7        | 0.11          |
| (3,1361) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 7        | 0.11          |
| (3,1361) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 10       | 0.11          |
| (3,1361) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 10       | 0.11          |
| (3,1361) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 10       | 0.11          |
| (3,1361) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 15       | 0.11          |
| (3,1361) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 15       | 0.11          |
| (3,1361) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 15       | 0.11          |
| (3,1361) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 16       | 0.11          |
| (3,1361) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 16       | 0.11          |
| (3,1361) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 16       | 0.11          |
| (3,1361) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 22       | 0.11          |
| (3,1361) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 22       | 0.11          |
| (3,1361) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 22       | 0.11          |
| (3,1361) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 27       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1361) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 27       | 0.11          |
| (3,1361) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 27       | 0.11          |
| (3,1361) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 28       | 0.11          |
| (3,1361) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 28       | 0.11          |
| (3,1361) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 28       | 0.11          |
| (3,1361) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 29       | 0.11          |
| (3,1361) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 29       | 0.11          |
| (3,1361) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 29       | 0.11          |
| (3,1361) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 37       | 0.11          |
| (3,1361) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 37       | 0.11          |
| (3,1361) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 37       | 0.11          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA   | 3        | 0.11          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA   | 3        | 0.11          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA   | 3        | 0.11          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA   | 6        | 0.11          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA   | 6        | 0.11          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA   | 6        | 0.11          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA   | 14       | 0.11          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA   | 14       | 0.11          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA   | 14       | 0.11          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA   | 15       | 0.11          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA   | 15       | 0.11          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA   | 15       | 0.11          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA   | 19       | 0.11          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA   | 19       | 0.11          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA   | 19       | 0.11          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA   | 20       | 0.11          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA   | 20       | 0.11          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA   | 20       | 0.11          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA   | 23       | 0.11          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA   | 23       | 0.11          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA   | 23       | 0.11          |
| (3,1347) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA   | 40       | 0.11          |
| (3,1347) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA   | 40       | 0.11          |
| (3,1347) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA   | 40       | 0.11          |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 7        | 0.11          |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 8        | 0.11          |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 14       | 0.11          |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 21       | 0.11          |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 25       | 0.11          |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 30       | 0.11          |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 33       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 37       | 0.11          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 22       | 0.11          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 22       | 0.11          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 22       | 0.11          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 32       | 0.11          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 32       | 0.11          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 32       | 0.11          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 33       | 0.11          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 33       | 0.11          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 33       | 0.11          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 37       | 0.11          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 37       | 0.11          |
| (3,1295) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 37       | 0.11          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1  | 2        | 0.11          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2  | 2        | 0.11          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3  | 2        | 0.11          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1  | 2        | 0.11          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2  | 2        | 0.11          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3  | 2        | 0.11          |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1  | 2        | 0.11          |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2  | 2        | 0.11          |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3  | 2        | 0.11          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1  | 13       | 0.11          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2  | 13       | 0.11          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3  | 13       | 0.11          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1  | 13       | 0.11          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2  | 13       | 0.11          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3  | 13       | 0.11          |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1  | 13       | 0.11          |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2  | 13       | 0.11          |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3  | 13       | 0.11          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1  | 14       | 0.11          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2  | 14       | 0.11          |
| (3,1294) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3  | 14       | 0.11          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1  | 14       | 0.11          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2  | 14       | 0.11          |
| (3,1294) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3  | 14       | 0.11          |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1  | 14       | 0.11          |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2  | 14       | 0.11          |
| (3,1294) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3  | 14       | 0.11          |
| (3,1293) | 1:40:A:VAL:HG21 | 1:42:A:TRP:HE1  | 12       | 0.11          |
| (3,1293) | 1:40:A:VAL:HG22 | 1:42:A:TRP:HE1  | 12       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1293) | 1:40:A:VAL:HG23 | 1:42:A:TRP:HE1  | 12       | 0.11          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 22       | 0.11          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 22       | 0.11          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 22       | 0.11          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 32       | 0.11          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 32       | 0.11          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 32       | 0.11          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 33       | 0.11          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 33       | 0.11          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 33       | 0.11          |
| (3,1282) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 37       | 0.11          |
| (3,1282) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 37       | 0.11          |
| (3,1282) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 37       | 0.11          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 16       | 0.11          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 16       | 0.11          |
| (3,1272) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 16       | 0.11          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 16       | 0.11          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 16       | 0.11          |
| (3,1272) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 16       | 0.11          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 16       | 0.11          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 16       | 0.11          |
| (3,1272) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 16       | 0.11          |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 31       | 0.11          |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 31       | 0.11          |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 31       | 0.11          |
| (3,1265) | 1:67:A:THR:HG21 | 1:56:A:ASN:H    | 11       | 0.11          |
| (3,1265) | 1:67:A:THR:HG22 | 1:56:A:ASN:H    | 11       | 0.11          |
| (3,1265) | 1:67:A:THR:HG23 | 1:56:A:ASN:H    | 11       | 0.11          |
| (3,1265) | 1:67:A:THR:HG21 | 1:56:A:ASN:H    | 22       | 0.11          |
| (3,1265) | 1:67:A:THR:HG22 | 1:56:A:ASN:H    | 22       | 0.11          |
| (3,1265) | 1:67:A:THR:HG23 | 1:56:A:ASN:H    | 22       | 0.11          |
| (3,1265) | 1:67:A:THR:HG21 | 1:56:A:ASN:H    | 25       | 0.11          |
| (3,1265) | 1:67:A:THR:HG22 | 1:56:A:ASN:H    | 25       | 0.11          |
| (3,1265) | 1:67:A:THR:HG23 | 1:56:A:ASN:H    | 25       | 0.11          |
| (3,1265) | 1:67:A:THR:HG21 | 1:56:A:ASN:H    | 30       | 0.11          |
| (3,1265) | 1:67:A:THR:HG22 | 1:56:A:ASN:H    | 30       | 0.11          |
| (3,1265) | 1:67:A:THR:HG23 | 1:56:A:ASN:H    | 30       | 0.11          |
| (3,1252) | 1:28:A:THR:HG21 | 1:67:A:THR:HG21 | 34       | 0.11          |
| (3,1252) | 1:28:A:THR:HG21 | 1:67:A:THR:HG22 | 34       | 0.11          |
| (3,1252) | 1:28:A:THR:HG21 | 1:67:A:THR:HG23 | 34       | 0.11          |
| (3,1252) | 1:28:A:THR:HG22 | 1:67:A:THR:HG21 | 34       | 0.11          |
| (3,1252) | 1:28:A:THR:HG22 | 1:67:A:THR:HG22 | 34       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1252) | 1:28:A:THR:HG22 | 1:67:A:THR:HG23 | 34       | 0.11          |
| (3,1252) | 1:28:A:THR:HG23 | 1:67:A:THR:HG21 | 34       | 0.11          |
| (3,1252) | 1:28:A:THR:HG23 | 1:67:A:THR:HG22 | 34       | 0.11          |
| (3,1252) | 1:28:A:THR:HG23 | 1:67:A:THR:HG23 | 34       | 0.11          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 4        | 0.11          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 4        | 0.11          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 4        | 0.11          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 11       | 0.11          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 11       | 0.11          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 11       | 0.11          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 16       | 0.11          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 16       | 0.11          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 16       | 0.11          |
| (3,1248) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 27       | 0.11          |
| (3,1248) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 27       | 0.11          |
| (3,1248) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 27       | 0.11          |
| (3,1243) | 1:13:A:THR:HG21 | 1:34:A:SER:H    | 7        | 0.11          |
| (3,1243) | 1:13:A:THR:HG22 | 1:34:A:SER:H    | 7        | 0.11          |
| (3,1243) | 1:13:A:THR:HG23 | 1:34:A:SER:H    | 7        | 0.11          |
| (3,1243) | 1:13:A:THR:HG21 | 1:34:A:SER:H    | 40       | 0.11          |
| (3,1243) | 1:13:A:THR:HG22 | 1:34:A:SER:H    | 40       | 0.11          |
| (3,1243) | 1:13:A:THR:HG23 | 1:34:A:SER:H    | 40       | 0.11          |
| (3,1240) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3  | 2        | 0.11          |
| (3,1240) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3  | 2        | 0.11          |
| (3,1240) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3  | 2        | 0.11          |
| (3,1240) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3  | 12       | 0.11          |
| (3,1240) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3  | 12       | 0.11          |
| (3,1240) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3  | 12       | 0.11          |
| (3,1240) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3  | 19       | 0.11          |
| (3,1240) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3  | 19       | 0.11          |
| (3,1240) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3  | 19       | 0.11          |
| (3,1230) | 1:101:A:LEU:H   | 1:22:A:SER:HA   | 3        | 0.11          |
| (3,1230) | 1:101:A:LEU:H   | 1:22:A:SER:HA   | 13       | 0.11          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 2        | 0.11          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 2        | 0.11          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 2        | 0.11          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 5        | 0.11          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 5        | 0.11          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 5        | 0.11          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 21       | 0.11          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 21       | 0.11          |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 21       | 0.11          |

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| Key      | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|----------|--------------|-----------------|----------|---------------|
| (3,1226) | 1:97:A:LEU:H | 1:97:A:LEU:HD21 | 24       | 0.11          |
| (3,1226) | 1:97:A:LEU:H | 1:97:A:LEU:HD22 | 24       | 0.11          |
| (3,1226) | 1:97:A:LEU:H | 1:97:A:LEU:HD23 | 24       | 0.11          |
| (3,1226) | 1:97:A:LEU:H | 1:97:A:LEU:HD21 | 30       | 0.11          |
| (3,1226) | 1:97:A:LEU:H | 1:97:A:LEU:HD22 | 30       | 0.11          |
| (3,1226) | 1:97:A:LEU:H | 1:97:A:LEU:HD23 | 30       | 0.11          |
| (3,1226) | 1:97:A:LEU:H | 1:97:A:LEU:HD21 | 31       | 0.11          |
| (3,1226) | 1:97:A:LEU:H | 1:97:A:LEU:HD22 | 31       | 0.11          |
| (3,1226) | 1:97:A:LEU:H | 1:97:A:LEU:HD23 | 31       | 0.11          |
| (3,1226) | 1:97:A:LEU:H | 1:97:A:LEU:HD21 | 32       | 0.11          |
| (3,1226) | 1:97:A:LEU:H | 1:97:A:LEU:HD22 | 32       | 0.11          |
| (3,1226) | 1:97:A:LEU:H | 1:97:A:LEU:HD23 | 32       | 0.11          |
| (3,1226) | 1:97:A:LEU:H | 1:97:A:LEU:HD21 | 33       | 0.11          |
| (3,1226) | 1:97:A:LEU:H | 1:97:A:LEU:HD22 | 33       | 0.11          |
| (3,1226) | 1:97:A:LEU:H | 1:97:A:LEU:HD23 | 33       | 0.11          |
| (3,1226) | 1:97:A:LEU:H | 1:97:A:LEU:HD21 | 35       | 0.11          |
| (3,1226) | 1:97:A:LEU:H | 1:97:A:LEU:HD22 | 35       | 0.11          |
| (3,1226) | 1:97:A:LEU:H | 1:97:A:LEU:HD23 | 35       | 0.11          |
| (3,1226) | 1:97:A:LEU:H | 1:97:A:LEU:HD21 | 36       | 0.11          |
| (3,1226) | 1:97:A:LEU:H | 1:97:A:LEU:HD22 | 36       | 0.11          |
| (3,1226) | 1:97:A:LEU:H | 1:97:A:LEU:HD23 | 36       | 0.11          |
| (3,1226) | 1:97:A:LEU:H | 1:97:A:LEU:HD21 | 38       | 0.11          |
| (3,1226) | 1:97:A:LEU:H | 1:97:A:LEU:HD22 | 38       | 0.11          |
| (3,1226) | 1:97:A:LEU:H | 1:97:A:LEU:HD23 | 38       | 0.11          |
| (3,1221) | 1:69:A:HIS:H | 1:56:A:ASN:H    | 31       | 0.11          |
| (3,1221) | 1:69:A:HIS:H | 1:56:A:ASN:H    | 34       | 0.11          |
| (3,1221) | 1:69:A:HIS:H | 1:56:A:ASN:H    | 40       | 0.11          |
| (3,1217) | 1:66:A:MET:H | 1:28:A:THR:HA   | 8        | 0.11          |
| (3,1217) | 1:66:A:MET:H | 1:28:A:THR:HA   | 9        | 0.11          |
| (3,1217) | 1:66:A:MET:H | 1:28:A:THR:HA   | 30       | 0.11          |
| (3,1217) | 1:66:A:MET:H | 1:28:A:THR:HA   | 33       | 0.11          |
| (3,1217) | 1:66:A:MET:H | 1:28:A:THR:HA   | 34       | 0.11          |
| (3,1217) | 1:66:A:MET:H | 1:28:A:THR:HA   | 40       | 0.11          |
| (3,1212) | 1:56:A:ASN:H | 1:66:A:MET:HG2  | 32       | 0.11          |
| (3,1208) | 1:42:A:TRP:H | 1:57:A:PHE:HE1  | 7        | 0.11          |
| (3,1208) | 1:42:A:TRP:H | 1:57:A:PHE:HE2  | 7        | 0.11          |
| (3,1208) | 1:42:A:TRP:H | 1:57:A:PHE:HE1  | 29       | 0.11          |
| (3,1208) | 1:42:A:TRP:H | 1:57:A:PHE:HE2  | 29       | 0.11          |
| (3,1208) | 1:42:A:TRP:H | 1:57:A:PHE:HE1  | 39       | 0.11          |
| (3,1208) | 1:42:A:TRP:H | 1:57:A:PHE:HE2  | 39       | 0.11          |
| (3,1201) | 1:33:A:VAL:H | 1:63:A:CYS:HA   | 4        | 0.11          |
| (3,1180) | 1:47:A:THR:H | 1:44:A:LYS:HB3  | 3        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1180) | 1:47:A:THR:H    | 1:44:A:LYS:HB3  | 22       | 0.11          |
| (3,1180) | 1:47:A:THR:H    | 1:44:A:LYS:HB3  | 24       | 0.11          |
| (3,1180) | 1:47:A:THR:H    | 1:44:A:LYS:HB3  | 40       | 0.11          |
| (3,1152) | 1:54:A:LYS:H    | 1:53:A:GLN:HG3  | 4        | 0.11          |
| (3,1152) | 1:54:A:LYS:H    | 1:53:A:GLN:HG3  | 13       | 0.11          |
| (3,1152) | 1:54:A:LYS:H    | 1:53:A:GLN:HG3  | 39       | 0.11          |
| (3,1152) | 1:54:A:LYS:H    | 1:53:A:GLN:HG3  | 40       | 0.11          |
| (3,1131) | 1:40:A:VAL:H    | 1:83:A:ALA:HB1  | 7        | 0.11          |
| (3,1131) | 1:40:A:VAL:H    | 1:83:A:ALA:HB2  | 7        | 0.11          |
| (3,1131) | 1:40:A:VAL:H    | 1:83:A:ALA:HB3  | 7        | 0.11          |
| (3,1063) | 1:71:A:VAL:H    | 1:25:A:GLN:H    | 5        | 0.11          |
| (3,1051) | 1:26:A:SER:H    | 1:25:A:GLN:HG2  | 17       | 0.11          |
| (3,1036) | 1:56:A:ASN:HD22 | 1:56:A:ASN:HA   | 7        | 0.11          |
| (3,1019) | 1:48:A:GLU:H    | 1:48:A:GLU:HG3  | 1        | 0.11          |
| (3,1019) | 1:48:A:GLU:H    | 1:48:A:GLU:HG3  | 4        | 0.11          |
| (3,1019) | 1:48:A:GLU:H    | 1:48:A:GLU:HG3  | 23       | 0.11          |
| (3,1019) | 1:48:A:GLU:H    | 1:48:A:GLU:HG3  | 26       | 0.11          |
| (3,998)  | 1:79:A:TYR:H    | 1:94:A:THR:HG21 | 3        | 0.11          |
| (3,998)  | 1:79:A:TYR:H    | 1:94:A:THR:HG22 | 3        | 0.11          |
| (3,998)  | 1:79:A:TYR:H    | 1:94:A:THR:HG23 | 3        | 0.11          |
| (3,998)  | 1:79:A:TYR:H    | 1:94:A:THR:HG21 | 4        | 0.11          |
| (3,998)  | 1:79:A:TYR:H    | 1:94:A:THR:HG22 | 4        | 0.11          |
| (3,998)  | 1:79:A:TYR:H    | 1:94:A:THR:HG23 | 4        | 0.11          |
| (3,998)  | 1:79:A:TYR:H    | 1:94:A:THR:HG21 | 15       | 0.11          |
| (3,998)  | 1:79:A:TYR:H    | 1:94:A:THR:HG22 | 15       | 0.11          |
| (3,998)  | 1:79:A:TYR:H    | 1:94:A:THR:HG23 | 15       | 0.11          |
| (3,998)  | 1:79:A:TYR:H    | 1:94:A:THR:HG21 | 22       | 0.11          |
| (3,998)  | 1:79:A:TYR:H    | 1:94:A:THR:HG22 | 22       | 0.11          |
| (3,998)  | 1:79:A:TYR:H    | 1:94:A:THR:HG23 | 22       | 0.11          |
| (3,998)  | 1:79:A:TYR:H    | 1:94:A:THR:HG21 | 25       | 0.11          |
| (3,998)  | 1:79:A:TYR:H    | 1:94:A:THR:HG22 | 25       | 0.11          |
| (3,998)  | 1:79:A:TYR:H    | 1:94:A:THR:HG23 | 25       | 0.11          |
| (3,998)  | 1:79:A:TYR:H    | 1:94:A:THR:HG21 | 30       | 0.11          |
| (3,998)  | 1:79:A:TYR:H    | 1:94:A:THR:HG22 | 30       | 0.11          |
| (3,998)  | 1:79:A:TYR:H    | 1:94:A:THR:HG23 | 30       | 0.11          |
| (3,988)  | 1:12:A:PHE:H    | 1:11:A:GLN:HB2  | 3        | 0.11          |
| (3,988)  | 1:12:A:PHE:H    | 1:11:A:GLN:HB2  | 4        | 0.11          |
| (3,988)  | 1:12:A:PHE:H    | 1:11:A:GLN:HB2  | 8        | 0.11          |
| (3,988)  | 1:12:A:PHE:H    | 1:11:A:GLN:HB2  | 14       | 0.11          |
| (3,988)  | 1:12:A:PHE:H    | 1:11:A:GLN:HB2  | 15       | 0.11          |
| (3,988)  | 1:12:A:PHE:H    | 1:11:A:GLN:HB2  | 17       | 0.11          |
| (3,968)  | 1:21:A:VAL:H    | 1:99:A:GLY:HA3  | 14       | 0.11          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 16       | 0.11          |
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 27       | 0.11          |
| (3,968) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 28       | 0.11          |
| (3,942) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 12       | 0.11          |
| (3,942) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 17       | 0.11          |
| (3,942) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 18       | 0.11          |
| (3,942) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 24       | 0.11          |
| (3,942) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 26       | 0.11          |
| (3,942) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 36       | 0.11          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 3        | 0.11          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 3        | 0.11          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 3        | 0.11          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 6        | 0.11          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 6        | 0.11          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 6        | 0.11          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 8        | 0.11          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 8        | 0.11          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 8        | 0.11          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 16       | 0.11          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 16       | 0.11          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 16       | 0.11          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 25       | 0.11          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 25       | 0.11          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 25       | 0.11          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 29       | 0.11          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 29       | 0.11          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 29       | 0.11          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 32       | 0.11          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 32       | 0.11          |
| (3,934) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 32       | 0.11          |
| (3,900) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 3        | 0.11          |
| (3,900) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 10       | 0.11          |
| (3,900) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 13       | 0.11          |
| (3,900) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 15       | 0.11          |
| (3,900) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 18       | 0.11          |
| (3,900) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 26       | 0.11          |
| (3,900) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 27       | 0.11          |
| (3,900) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 29       | 0.11          |
| (3,900) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 32       | 0.11          |
| (3,900) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 35       | 0.11          |
| (3,900) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 37       | 0.11          |
| (3,890) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 2        | 0.11          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,890) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 5        | 0.11          |
| (3,890) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 11       | 0.11          |
| (3,890) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 12       | 0.11          |
| (3,890) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 17       | 0.11          |
| (3,890) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 19       | 0.11          |
| (3,890) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 25       | 0.11          |
| (3,890) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 26       | 0.11          |
| (3,890) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 36       | 0.11          |
| (3,889) | 1:80:A:SER:H | 1:43:A:TYR:HB3  | 38       | 0.11          |
| (3,880) | 1:30:A:GLU:H | 1:29:A:PHE:HB2  | 12       | 0.11          |
| (3,863) | 1:86:A:GLU:H | 1:85:A:LEU:HB3  | 29       | 0.11          |
| (3,863) | 1:86:A:GLU:H | 1:85:A:LEU:HB3  | 34       | 0.11          |
| (3,860) | 1:86:A:GLU:H | 1:85:A:LEU:HA   | 3        | 0.11          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 11       | 0.11          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 11       | 0.11          |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 11       | 0.11          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 17       | 0.11          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 17       | 0.11          |
| (3,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 17       | 0.11          |
| (3,813) | 1:25:A:GLN:H | 1:25:A:GLN:HG3  | 4        | 0.11          |
| (3,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB   | 13       | 0.11          |
| (3,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB   | 19       | 0.11          |
| (3,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB   | 25       | 0.11          |
| (3,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB   | 27       | 0.11          |
| (3,742) | 1:76:A:GLU:H | 1:77:A:GLY:H    | 3        | 0.11          |
| (3,742) | 1:76:A:GLU:H | 1:77:A:GLY:H    | 10       | 0.11          |
| (3,742) | 1:76:A:GLU:H | 1:77:A:GLY:H    | 14       | 0.11          |
| (3,742) | 1:76:A:GLU:H | 1:77:A:GLY:H    | 16       | 0.11          |
| (3,742) | 1:76:A:GLU:H | 1:77:A:GLY:H    | 17       | 0.11          |
| (3,726) | 1:49:A:LEU:H | 1:48:A:GLU:HG3  | 4        | 0.11          |
| (3,726) | 1:49:A:LEU:H | 1:48:A:GLU:HG3  | 5        | 0.11          |
| (3,726) | 1:49:A:LEU:H | 1:48:A:GLU:HG3  | 19       | 0.11          |
| (3,726) | 1:49:A:LEU:H | 1:48:A:GLU:HG3  | 21       | 0.11          |
| (3,726) | 1:49:A:LEU:H | 1:48:A:GLU:HG3  | 32       | 0.11          |
| (3,726) | 1:49:A:LEU:H | 1:48:A:GLU:HG3  | 34       | 0.11          |
| (3,726) | 1:49:A:LEU:H | 1:48:A:GLU:HG3  | 36       | 0.11          |
| (3,709) | 1:16:A:ILE:H | 1:31:A:CYS:HB2  | 11       | 0.11          |
| (3,709) | 1:16:A:ILE:H | 1:31:A:CYS:HB2  | 14       | 0.11          |
| (3,709) | 1:16:A:ILE:H | 1:31:A:CYS:HB2  | 25       | 0.11          |
| (3,709) | 1:16:A:ILE:H | 1:31:A:CYS:HB2  | 35       | 0.11          |
| (3,666) | 1:72:A:THR:H | 1:72:A:THR:HB   | 2        | 0.11          |
| (3,666) | 1:72:A:THR:H | 1:72:A:THR:HB   | 3        | 0.11          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (3,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 4        | 0.11          |
| (3,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 5        | 0.11          |
| (3,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 6        | 0.11          |
| (3,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 11       | 0.11          |
| (3,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 12       | 0.11          |
| (3,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 13       | 0.11          |
| (3,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 14       | 0.11          |
| (3,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 15       | 0.11          |
| (3,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 16       | 0.11          |
| (3,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 21       | 0.11          |
| (3,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 22       | 0.11          |
| (3,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 25       | 0.11          |
| (3,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 26       | 0.11          |
| (3,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 32       | 0.11          |
| (3,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 37       | 0.11          |
| (3,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 38       | 0.11          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 1        | 0.11          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 3        | 0.11          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 8        | 0.11          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 21       | 0.11          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 25       | 0.11          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 28       | 0.11          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 31       | 0.11          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 32       | 0.11          |
| (3,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 38       | 0.11          |
| (3,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 22       | 0.11          |
| (3,609) | 1:43:A:TYR:H  | 1:42:A:TRP:HB2  | 10       | 0.11          |
| (3,595) | 1:3:A:ASP:H   | 1:2:A:ILE:HG21  | 14       | 0.11          |
| (3,595) | 1:3:A:ASP:H   | 1:2:A:ILE:HG22  | 14       | 0.11          |
| (3,595) | 1:3:A:ASP:H   | 1:2:A:ILE:HG23  | 14       | 0.11          |
| (3,589) | 1:93:A:SER:H  | 1:92:A:ARG:HG2  | 7        | 0.11          |
| (3,589) | 1:93:A:SER:H  | 1:92:A:ARG:HG2  | 33       | 0.11          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 9        | 0.11          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 9        | 0.11          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 9        | 0.11          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 17       | 0.11          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 17       | 0.11          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 17       | 0.11          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 28       | 0.11          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 28       | 0.11          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 28       | 0.11          |
| (3,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 29       | 0.11          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 29       | 0.11          |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 29       | 0.11          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1  | 18       | 0.11          |
| (3,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2  | 18       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 2        | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 2        | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 2        | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 4        | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 4        | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 4        | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 5        | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 5        | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 5        | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 7        | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 7        | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 7        | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 8        | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 8        | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 8        | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 10       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 10       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 10       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 13       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 13       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 13       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 14       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 14       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 14       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 15       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 15       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 15       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 17       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 17       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 17       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 21       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 21       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 21       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 22       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 22       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 22       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 24       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 24       | 0.11          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 24       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 25       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 25       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 25       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 26       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 26       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 26       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 28       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 28       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 28       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 30       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 30       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 30       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 31       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 31       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 31       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 32       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 32       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 32       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 34       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 34       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 34       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 36       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 36       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 36       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 37       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 37       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 37       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 38       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 38       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 38       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 39       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 39       | 0.11          |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 39       | 0.11          |
| (3,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 26       | 0.11          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 2        | 0.11          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 3        | 0.11          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 6        | 0.11          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 9        | 0.11          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 10       | 0.11          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 11       | 0.11          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 15       | 0.11          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 19       | 0.11          |
| (3,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 28       | 0.11          |
| (3,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 9        | 0.11          |
| (3,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 9        | 0.11          |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 5        | 0.11          |
| (3,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 7        | 0.11          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 2        | 0.11          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 7        | 0.11          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 12       | 0.11          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 16       | 0.11          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 24       | 0.11          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 33       | 0.11          |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 40       | 0.11          |
| (3,419) | 1:69:A:HIS:H | 1:54:A:LYS:HA   | 40       | 0.11          |
| (3,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD21 | 22       | 0.11          |
| (3,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD22 | 22       | 0.11          |
| (3,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD23 | 22       | 0.11          |
| (3,393) | 1:77:A:GLY:H | 1:96:A:GLU:HA   | 14       | 0.11          |
| (3,393) | 1:77:A:GLY:H | 1:96:A:GLU:HA   | 28       | 0.11          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 7        | 0.11          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 7        | 0.11          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 7        | 0.11          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 9        | 0.11          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 9        | 0.11          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 9        | 0.11          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 21       | 0.11          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 21       | 0.11          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 21       | 0.11          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 37       | 0.11          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 37       | 0.11          |
| (3,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 37       | 0.11          |
| (3,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 13       | 0.11          |
| (3,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 14       | 0.11          |
| (3,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 16       | 0.11          |
| (3,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 20       | 0.11          |
| (3,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 21       | 0.11          |
| (3,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 30       | 0.11          |
| (3,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 33       | 0.11          |
| (3,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD1  | 8        | 0.11          |
| (3,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD2  | 8        | 0.11          |
| (3,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD1  | 20       | 0.11          |
| (3,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD2  | 20       | 0.11          |

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| Key     | Atom-1       | Atom-2         | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (3,314) | 1:63:A:CYS:H | 1:64:A:HIS:HD2 | 8        | 0.11          |
| (3,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3 | 12       | 0.11          |
| (3,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3 | 29       | 0.11          |
| (3,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3 | 38       | 0.11          |
| (3,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3 | 2        | 0.11          |
| (3,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3 | 4        | 0.11          |
| (3,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3 | 9        | 0.11          |
| (3,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3 | 16       | 0.11          |
| (3,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3 | 27       | 0.11          |
| (3,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3 | 31       | 0.11          |
| (3,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3 | 37       | 0.11          |
| (3,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 3        | 0.11          |
| (3,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 4        | 0.11          |
| (3,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 5        | 0.11          |
| (3,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 8        | 0.11          |
| (3,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 14       | 0.11          |
| (3,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 17       | 0.11          |
| (3,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 18       | 0.11          |
| (3,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 26       | 0.11          |
| (3,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 29       | 0.11          |
| (3,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 30       | 0.11          |
| (3,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 31       | 0.11          |
| (3,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 32       | 0.11          |
| (3,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 34       | 0.11          |
| (3,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 35       | 0.11          |
| (3,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 37       | 0.11          |
| (3,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 40       | 0.11          |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1 | 3        | 0.11          |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2 | 3        | 0.11          |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1 | 14       | 0.11          |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2 | 14       | 0.11          |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1 | 15       | 0.11          |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2 | 15       | 0.11          |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1 | 19       | 0.11          |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2 | 19       | 0.11          |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1 | 22       | 0.11          |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2 | 22       | 0.11          |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1 | 28       | 0.11          |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2 | 28       | 0.11          |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1 | 32       | 0.11          |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2 | 32       | 0.11          |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1 | 33       | 0.11          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD2  | 33       | 0.11          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD1  | 35       | 0.11          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD2  | 35       | 0.11          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD1  | 40       | 0.11          |
| (3,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD2  | 40       | 0.11          |
| (3,203) | 1:90:A:GLU:H  | 1:91:A:ALA:H    | 1        | 0.11          |
| (3,203) | 1:90:A:GLU:H  | 1:91:A:ALA:H    | 4        | 0.11          |
| (3,203) | 1:90:A:GLU:H  | 1:91:A:ALA:H    | 5        | 0.11          |
| (3,203) | 1:90:A:GLU:H  | 1:91:A:ALA:H    | 8        | 0.11          |
| (3,203) | 1:90:A:GLU:H  | 1:91:A:ALA:H    | 9        | 0.11          |
| (3,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 11       | 0.11          |
| (3,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 18       | 0.11          |
| (3,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 34       | 0.11          |
| (3,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 38       | 0.11          |
| (3,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 39       | 0.11          |
| (3,198) | 1:90:A:GLU:H  | 1:90:A:GLU:HB2  | 15       | 0.11          |
| (3,182) | 1:11:A:GLN:H  | 1:10:A:ILE:HD11 | 1        | 0.11          |
| (3,182) | 1:11:A:GLN:H  | 1:10:A:ILE:HD12 | 1        | 0.11          |
| (3,182) | 1:11:A:GLN:H  | 1:10:A:ILE:HD13 | 1        | 0.11          |
| (3,182) | 1:11:A:GLN:H  | 1:10:A:ILE:HD11 | 3        | 0.11          |
| (3,182) | 1:11:A:GLN:H  | 1:10:A:ILE:HD12 | 3        | 0.11          |
| (3,182) | 1:11:A:GLN:H  | 1:10:A:ILE:HD13 | 3        | 0.11          |
| (3,182) | 1:11:A:GLN:H  | 1:10:A:ILE:HD11 | 8        | 0.11          |
| (3,182) | 1:11:A:GLN:H  | 1:10:A:ILE:HD12 | 8        | 0.11          |
| (3,182) | 1:11:A:GLN:H  | 1:10:A:ILE:HD13 | 8        | 0.11          |
| (3,182) | 1:11:A:GLN:H  | 1:10:A:ILE:HD11 | 20       | 0.11          |
| (3,182) | 1:11:A:GLN:H  | 1:10:A:ILE:HD12 | 20       | 0.11          |
| (3,182) | 1:11:A:GLN:H  | 1:10:A:ILE:HD13 | 20       | 0.11          |
| (3,165) | 1:10:A:ILE:H  | 1:9:A:PRO:HB2   | 8        | 0.11          |
| (3,165) | 1:10:A:ILE:H  | 1:9:A:PRO:HB2   | 9        | 0.11          |
| (3,165) | 1:10:A:ILE:H  | 1:9:A:PRO:HB2   | 11       | 0.11          |
| (3,165) | 1:10:A:ILE:H  | 1:9:A:PRO:HB2   | 13       | 0.11          |
| (3,165) | 1:10:A:ILE:H  | 1:9:A:PRO:HB2   | 17       | 0.11          |
| (3,144) | 1:101:A:LEU:H | 1:100:A:GLU:HB2 | 39       | 0.11          |
| (3,113) | 1:63:A:CYS:H  | 1:60:A:ASP:H    | 9        | 0.11          |
| (3,113) | 1:63:A:CYS:H  | 1:60:A:ASP:H    | 31       | 0.11          |
| (3,57)  | 1:42:A:TRP:H  | 1:42:A:TRP:HB3  | 1        | 0.11          |
| (3,57)  | 1:42:A:TRP:H  | 1:42:A:TRP:HB3  | 5        | 0.11          |
| (3,57)  | 1:42:A:TRP:H  | 1:42:A:TRP:HB3  | 18       | 0.11          |
| (3,57)  | 1:42:A:TRP:H  | 1:42:A:TRP:HB3  | 22       | 0.11          |
| (3,57)  | 1:42:A:TRP:H  | 1:42:A:TRP:HB3  | 34       | 0.11          |
| (3,51)  | 1:57:A:PHE:H  | 1:56:A:ASN:HB2  | 4        | 0.11          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,51)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2  | 19       | 0.11          |
| (3,39)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3  | 29       | 0.11          |
| (3,24)   | 1:89:A:GLY:H   | 1:9:A:PRO:HB3   | 16       | 0.11          |
| (1,3211) | 1:69:A:HIS:HE1 | 1:67:A:THR:HB   | 24       | 0.11          |
| (1,3211) | 1:69:A:HIS:HE1 | 1:67:A:THR:HB   | 28       | 0.11          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 5        | 0.11          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 5        | 0.11          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 11       | 0.11          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 11       | 0.11          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 13       | 0.11          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 13       | 0.11          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 20       | 0.11          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 20       | 0.11          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 23       | 0.11          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 23       | 0.11          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 26       | 0.11          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 26       | 0.11          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 30       | 0.11          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 30       | 0.11          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 31       | 0.11          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 31       | 0.11          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 37       | 0.11          |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 37       | 0.11          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 25       | 0.11          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 25       | 0.11          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 25       | 0.11          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 25       | 0.11          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 25       | 0.11          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 25       | 0.11          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 32       | 0.11          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 32       | 0.11          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 32       | 0.11          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 32       | 0.11          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 32       | 0.11          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 32       | 0.11          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD21 | 34       | 0.11          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD22 | 34       | 0.11          |
| (1,3200) | 1:55:A:TYR:HD1 | 1:49:A:LEU:HD23 | 34       | 0.11          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD21 | 34       | 0.11          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD22 | 34       | 0.11          |
| (1,3200) | 1:55:A:TYR:HD2 | 1:49:A:LEU:HD23 | 34       | 0.11          |
| (1,3197) | 1:42:A:TRP:HZ2 | 1:30:A:GLU:HA   | 1        | 0.11          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3197) | 1:42:A:TRP:HZ2 | 1:30:A:GLU:HA   | 18       | 0.11          |
| (1,3197) | 1:42:A:TRP:HZ2 | 1:30:A:GLU:HA   | 28       | 0.11          |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG21 | 9        | 0.11          |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG22 | 9        | 0.11          |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG23 | 9        | 0.11          |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG21 | 22       | 0.11          |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG22 | 22       | 0.11          |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG23 | 22       | 0.11          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 13       | 0.11          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 13       | 0.11          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 13       | 0.11          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 13       | 0.11          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 14       | 0.11          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 14       | 0.11          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 14       | 0.11          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 14       | 0.11          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 34       | 0.11          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 34       | 0.11          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 34       | 0.11          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 34       | 0.11          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE1  | 37       | 0.11          |
| (1,3190) | 1:79:A:TYR:HD1 | 1:29:A:PHE:HE2  | 37       | 0.11          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE1  | 37       | 0.11          |
| (1,3190) | 1:79:A:TYR:HD2 | 1:29:A:PHE:HE2  | 37       | 0.11          |
| (1,3185) | 1:43:A:TYR:HD1 | 1:44:A:LYS:H    | 31       | 0.11          |
| (1,3185) | 1:43:A:TYR:HD2 | 1:44:A:LYS:H    | 31       | 0.11          |
| (1,3177) | 1:42:A:TRP:HE1 | 1:81:A:VAL:HB   | 29       | 0.11          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 2        | 0.11          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 2        | 0.11          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 2        | 0.11          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 4        | 0.11          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 4        | 0.11          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 4        | 0.11          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 14       | 0.11          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 14       | 0.11          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 14       | 0.11          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 23       | 0.11          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 23       | 0.11          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 23       | 0.11          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 24       | 0.11          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 24       | 0.11          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 24       | 0.11          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 32       | 0.11          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 32       | 0.11          |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 32       | 0.11          |
| (1,3169) | 1:69:A:HIS:HD2 | 1:69:A:HIS:HB3  | 14       | 0.11          |
| (1,3158) | 1:42:A:TRP:HD1 | 1:41:A:THR:HA   | 39       | 0.11          |
| (1,3137) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3  | 10       | 0.11          |
| (1,3137) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 10       | 0.11          |
| (1,3137) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3  | 14       | 0.11          |
| (1,3137) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 14       | 0.11          |
| (1,3137) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3  | 18       | 0.11          |
| (1,3137) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 18       | 0.11          |
| (1,3137) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3  | 26       | 0.11          |
| (1,3137) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 26       | 0.11          |
| (1,3137) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3  | 38       | 0.11          |
| (1,3137) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 38       | 0.11          |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2  | 1        | 0.11          |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2  | 1        | 0.11          |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2  | 3        | 0.11          |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2  | 3        | 0.11          |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2  | 5        | 0.11          |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2  | 5        | 0.11          |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2  | 13       | 0.11          |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2  | 13       | 0.11          |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2  | 22       | 0.11          |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2  | 22       | 0.11          |
| (1,3133) | 1:65:A:TYR:HE1 | 1:60:A:ASP:HB3  | 20       | 0.11          |
| (1,3133) | 1:65:A:TYR:HE2 | 1:60:A:ASP:HB3  | 20       | 0.11          |
| (1,3133) | 1:65:A:TYR:HE1 | 1:60:A:ASP:HB3  | 30       | 0.11          |
| (1,3133) | 1:65:A:TYR:HE2 | 1:60:A:ASP:HB3  | 30       | 0.11          |
| (1,3133) | 1:65:A:TYR:HE1 | 1:60:A:ASP:HB3  | 33       | 0.11          |
| (1,3133) | 1:65:A:TYR:HE2 | 1:60:A:ASP:HB3  | 33       | 0.11          |
| (1,3132) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB2  | 30       | 0.11          |
| (1,3132) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB2  | 30       | 0.11          |
| (1,3131) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3  | 31       | 0.11          |
| (1,3131) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3  | 31       | 0.11          |
| (1,3131) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3  | 40       | 0.11          |
| (1,3131) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3  | 40       | 0.11          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 6        | 0.11          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 6        | 0.11          |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 6        | 0.11          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 6        | 0.11          |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 6        | 0.11          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 6        | 0.11          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 3        | 0.11          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 3        | 0.11          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 3        | 0.11          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 3        | 0.11          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 3        | 0.11          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 3        | 0.11          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 5        | 0.11          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 5        | 0.11          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 5        | 0.11          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 5        | 0.11          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 5        | 0.11          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 5        | 0.11          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 10       | 0.11          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 10       | 0.11          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 10       | 0.11          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 10       | 0.11          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 10       | 0.11          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 10       | 0.11          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 19       | 0.11          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 19       | 0.11          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 19       | 0.11          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 19       | 0.11          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 19       | 0.11          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 19       | 0.11          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 21       | 0.11          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 21       | 0.11          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 21       | 0.11          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 21       | 0.11          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 21       | 0.11          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 21       | 0.11          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 33       | 0.11          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 33       | 0.11          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 33       | 0.11          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 33       | 0.11          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 33       | 0.11          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 33       | 0.11          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 40       | 0.11          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 40       | 0.11          |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 40       | 0.11          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 40       | 0.11          |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 40       | 0.11          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 40       | 0.11          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 5        | 0.11          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 5        | 0.11          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 5        | 0.11          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 5        | 0.11          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 30       | 0.11          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 30       | 0.11          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 30       | 0.11          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 30       | 0.11          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 33       | 0.11          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 33       | 0.11          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 33       | 0.11          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 33       | 0.11          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 35       | 0.11          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 35       | 0.11          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 35       | 0.11          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 35       | 0.11          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 38       | 0.11          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 38       | 0.11          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 38       | 0.11          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 38       | 0.11          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 40       | 0.11          |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 40       | 0.11          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 40       | 0.11          |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 40       | 0.11          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 2        | 0.11          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 2        | 0.11          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 2        | 0.11          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 2        | 0.11          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 2        | 0.11          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 2        | 0.11          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 18       | 0.11          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 18       | 0.11          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 18       | 0.11          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 18       | 0.11          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 18       | 0.11          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 18       | 0.11          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 30       | 0.11          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 30       | 0.11          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 30       | 0.11          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 30       | 0.11          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 30       | 0.11          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 30       | 0.11          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 34       | 0.11          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 34       | 0.11          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 34       | 0.11          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 34       | 0.11          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 34       | 0.11          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 34       | 0.11          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 38       | 0.11          |
| (1,3092) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 38       | 0.11          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 38       | 0.11          |
| (1,3092) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 38       | 0.11          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 38       | 0.11          |
| (1,3092) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE2  | 38       | 0.11          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 9        | 0.11          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 9        | 0.11          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 9        | 0.11          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 12       | 0.11          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 12       | 0.11          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 12       | 0.11          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 21       | 0.11          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 21       | 0.11          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 21       | 0.11          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 22       | 0.11          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 22       | 0.11          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 22       | 0.11          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG21 | 38       | 0.11          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG22 | 38       | 0.11          |
| (1,3084) | 1:98:A:LYS:HD3 | 1:20:A:VAL:HG23 | 38       | 0.11          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 16       | 0.11          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 16       | 0.11          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 18       | 0.11          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 18       | 0.11          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 36       | 0.11          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 36       | 0.11          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE1  | 40       | 0.11          |
| (1,3082) | 1:97:A:LEU:HB3 | 1:29:A:PHE:HE2  | 40       | 0.11          |
| (1,3040) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG21 | 7        | 0.11          |
| (1,3040) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG22 | 7        | 0.11          |
| (1,3040) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG23 | 7        | 0.11          |
| (1,3040) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG21 | 14       | 0.11          |
| (1,3040) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG22 | 14       | 0.11          |
| (1,3040) | 1:55:A:TYR:HA  | 1:68:A:ILE:HG23 | 14       | 0.11          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3033) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE1  | 1        | 0.11          |
| (1,3033) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE2  | 1        | 0.11          |
| (1,3033) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE1  | 6        | 0.11          |
| (1,3033) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE2  | 6        | 0.11          |
| (1,3033) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE1  | 18       | 0.11          |
| (1,3033) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE2  | 18       | 0.11          |
| (1,3033) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE1  | 27       | 0.11          |
| (1,3033) | 1:44:A:LYS:HE2 | 1:79:A:TYR:HE2  | 27       | 0.11          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 5        | 0.11          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 5        | 0.11          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 13       | 0.11          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 13       | 0.11          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 17       | 0.11          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 17       | 0.11          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 21       | 0.11          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 21       | 0.11          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 33       | 0.11          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 33       | 0.11          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD1  | 35       | 0.11          |
| (1,3013) | 1:30:A:GLU:HG2 | 1:65:A:TYR:HD2  | 35       | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 6        | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 6        | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 6        | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 9        | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 9        | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 9        | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 10       | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 10       | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 10       | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 15       | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 15       | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 15       | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 16       | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 16       | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 16       | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 17       | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 17       | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 17       | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 20       | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG22 | 20       | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG23 | 20       | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3 | 1:28:A:THR:HG21 | 21       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG22 | 21       | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG23 | 21       | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG21 | 24       | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG22 | 24       | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG23 | 24       | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG21 | 29       | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG22 | 29       | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG23 | 29       | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG21 | 33       | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG22 | 33       | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG23 | 33       | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG21 | 39       | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG22 | 39       | 0.11          |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG23 | 39       | 0.11          |
| (1,3009) | 1:102:A:ARG:HD3 | 1:102:A:ARG:HB2 | 24       | 0.11          |
| (1,3009) | 1:102:A:ARG:HD3 | 1:102:A:ARG:HB2 | 28       | 0.11          |
| (1,3009) | 1:102:A:ARG:HD3 | 1:102:A:ARG:HB2 | 30       | 0.11          |
| (1,3004) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG21 | 12       | 0.11          |
| (1,3004) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG22 | 12       | 0.11          |
| (1,3004) | 1:25:A:GLN:HB3  | 1:21:A:VAL:HG23 | 12       | 0.11          |
| (1,2996) | 1:15:A:ARG:HG2  | 1:93:A:SER:HB3  | 3        | 0.11          |
| (1,2996) | 1:15:A:ARG:HG2  | 1:93:A:SER:HB3  | 29       | 0.11          |
| (1,2996) | 1:15:A:ARG:HG2  | 1:93:A:SER:HB3  | 34       | 0.11          |
| (1,2996) | 1:15:A:ARG:HG2  | 1:93:A:SER:HB3  | 37       | 0.11          |
| (1,2974) | 1:65:A:TYR:HA   | 1:42:A:TRP:HZ2  | 6        | 0.11          |
| (1,2974) | 1:65:A:TYR:HA   | 1:42:A:TRP:HZ2  | 9        | 0.11          |
| (1,2974) | 1:65:A:TYR:HA   | 1:42:A:TRP:HZ2  | 30       | 0.11          |
| (1,2974) | 1:65:A:TYR:HA   | 1:42:A:TRP:HZ2  | 35       | 0.11          |
| (1,2974) | 1:65:A:TYR:HA   | 1:42:A:TRP:HZ2  | 38       | 0.11          |
| (1,2949) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 9        | 0.11          |
| (1,2949) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 12       | 0.11          |
| (1,2949) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 27       | 0.11          |
| (1,2949) | 1:8:A:GLU:HG2   | 1:8:A:GLU:HA    | 40       | 0.11          |
| (1,2942) | 1:90:A:GLU:HA   | 1:84:A:ARG:HA   | 4        | 0.11          |
| (1,2942) | 1:90:A:GLU:HA   | 1:84:A:ARG:HA   | 8        | 0.11          |
| (1,2937) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD1  | 10       | 0.11          |
| (1,2937) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD2  | 10       | 0.11          |
| (1,2937) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD1  | 14       | 0.11          |
| (1,2937) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD2  | 14       | 0.11          |
| (1,2937) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD1  | 18       | 0.11          |
| (1,2937) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD2  | 18       | 0.11          |
| (1,2937) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD1  | 26       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2937) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD2  | 26       | 0.11          |
| (1,2937) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD1  | 38       | 0.11          |
| (1,2937) | 1:30:A:GLU:HB3  | 1:65:A:TYR:HD2  | 38       | 0.11          |
| (1,2931) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 6        | 0.11          |
| (1,2931) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 10       | 0.11          |
| (1,2931) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 21       | 0.11          |
| (1,2931) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 28       | 0.11          |
| (1,2931) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 37       | 0.11          |
| (1,2931) | 1:26:A:SER:HA   | 1:70:A:ASN:H    | 40       | 0.11          |
| (1,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HG3  | 6        | 0.11          |
| (1,2910) | 1:98:A:LYS:HE3  | 1:98:A:LYS:HG3  | 26       | 0.11          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 1        | 0.11          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 2        | 0.11          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 3        | 0.11          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 7        | 0.11          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 8        | 0.11          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 9        | 0.11          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 10       | 0.11          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 14       | 0.11          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 15       | 0.11          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 18       | 0.11          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 19       | 0.11          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 20       | 0.11          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 22       | 0.11          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 23       | 0.11          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 25       | 0.11          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 26       | 0.11          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 28       | 0.11          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 30       | 0.11          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 31       | 0.11          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 32       | 0.11          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 34       | 0.11          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 36       | 0.11          |
| (1,2887) | 1:14:A:LYS:HB3  | 1:14:A:LYS:HG3  | 37       | 0.11          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 5        | 0.11          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 9        | 0.11          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 19       | 0.11          |
| (1,2868) | 1:102:A:ARG:HB2 | 1:102:A:ARG:HG2 | 29       | 0.11          |
| (1,2841) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA   | 6        | 0.11          |
| (1,2841) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA   | 9        | 0.11          |
| (1,2841) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA   | 22       | 0.11          |
| (1,2841) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA   | 24       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2841) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA   | 25       | 0.11          |
| (1,2841) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA   | 31       | 0.11          |
| (1,2841) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA   | 32       | 0.11          |
| (1,2841) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA   | 33       | 0.11          |
| (1,2841) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA   | 36       | 0.11          |
| (1,2841) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA   | 37       | 0.11          |
| (1,2841) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA   | 38       | 0.11          |
| (1,2841) | 1:84:A:ARG:HG2  | 1:84:A:ARG:HA   | 40       | 0.11          |
| (1,2802) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HB2  | 7        | 0.11          |
| (1,2802) | 1:15:A:ARG:HD3  | 1:15:A:ARG:HB2  | 31       | 0.11          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 1        | 0.11          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 3        | 0.11          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 8        | 0.11          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 21       | 0.11          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 25       | 0.11          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 28       | 0.11          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 31       | 0.11          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 32       | 0.11          |
| (1,2785) | 1:100:A:GLU:HG2 | 1:100:A:GLU:H   | 38       | 0.11          |
| (1,2754) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 13       | 0.11          |
| (1,2754) | 1:90:A:GLU:HB3  | 1:91:A:ALA:H    | 29       | 0.11          |
| (1,2745) | 1:86:A:GLU:HG2  | 1:86:A:GLU:H    | 19       | 0.11          |
| (1,2745) | 1:86:A:GLU:HG3  | 1:86:A:GLU:H    | 19       | 0.11          |
| (1,2716) | 1:48:A:GLU:HA   | 1:41:A:THR:HG21 | 12       | 0.11          |
| (1,2716) | 1:48:A:GLU:HA   | 1:41:A:THR:HG22 | 12       | 0.11          |
| (1,2716) | 1:48:A:GLU:HA   | 1:41:A:THR:HG23 | 12       | 0.11          |
| (1,2715) | 1:48:A:GLU:HA   | 1:49:A:LEU:HG   | 26       | 0.11          |
| (1,2713) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 9        | 0.11          |
| (1,2713) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 11       | 0.11          |
| (1,2713) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 14       | 0.11          |
| (1,2713) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 20       | 0.11          |
| (1,2713) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 29       | 0.11          |
| (1,2713) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 35       | 0.11          |
| (1,2713) | 1:48:A:GLU:HA   | 1:48:A:GLU:HG3  | 39       | 0.11          |
| (1,2699) | 1:23:A:GLU:HA   | 1:24:A:HIS:HA   | 2        | 0.11          |
| (1,2699) | 1:23:A:GLU:HA   | 1:24:A:HIS:HA   | 5        | 0.11          |
| (1,2699) | 1:23:A:GLU:HA   | 1:24:A:HIS:HA   | 8        | 0.11          |
| (1,2699) | 1:23:A:GLU:HA   | 1:24:A:HIS:HA   | 12       | 0.11          |
| (1,2699) | 1:23:A:GLU:HA   | 1:24:A:HIS:HA   | 13       | 0.11          |
| (1,2699) | 1:23:A:GLU:HA   | 1:24:A:HIS:HA   | 19       | 0.11          |
| (1,2699) | 1:23:A:GLU:HA   | 1:24:A:HIS:HA   | 20       | 0.11          |
| (1,2699) | 1:23:A:GLU:HA   | 1:24:A:HIS:HA   | 23       | 0.11          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,2699) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA   | 24       | 0.11          |
| (1,2699) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA   | 28       | 0.11          |
| (1,2699) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA   | 31       | 0.11          |
| (1,2699) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA   | 36       | 0.11          |
| (1,2699) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA   | 38       | 0.11          |
| (1,2699) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA   | 39       | 0.11          |
| (1,2686) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 7        | 0.11          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 5        | 0.11          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 8        | 0.11          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 9        | 0.11          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 10       | 0.11          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 15       | 0.11          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 16       | 0.11          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 21       | 0.11          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 23       | 0.11          |
| (1,2679) | 1:53:A:GLN:HB2 | 1:53:A:GLN:HG2  | 24       | 0.11          |
| (1,2675) | 1:25:A:GLN:HG3 | 1:26:A:SER:H    | 9        | 0.11          |
| (1,2675) | 1:25:A:GLN:HG3 | 1:26:A:SER:H    | 17       | 0.11          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 13       | 0.11          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 13       | 0.11          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 13       | 0.11          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 18       | 0.11          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 18       | 0.11          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 18       | 0.11          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 35       | 0.11          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 35       | 0.11          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 35       | 0.11          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 38       | 0.11          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 38       | 0.11          |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 38       | 0.11          |
| (1,2649) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 13       | 0.11          |
| (1,2649) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 14       | 0.11          |
| (1,2649) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 16       | 0.11          |
| (1,2649) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 20       | 0.11          |
| (1,2649) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 21       | 0.11          |
| (1,2649) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 30       | 0.11          |
| (1,2649) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 33       | 0.11          |
| (1,2646) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3   | 25       | 0.11          |
| (1,2646) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3   | 26       | 0.11          |
| (1,2646) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3   | 29       | 0.11          |
| (1,2646) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3   | 30       | 0.11          |
| (1,2646) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3   | 31       | 0.11          |

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| Key      | Atom-1         | Atom-2        | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (1,2646) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3 | 37       | 0.11          |
| (1,2646) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3 | 38       | 0.11          |
| (1,2646) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3 | 39       | 0.11          |
| (1,2645) | 1:9:A:PRO:HB3  | 1:9:A:PRO:HD3 | 23       | 0.11          |
| (1,2609) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H  | 20       | 0.11          |
| (1,2609) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H  | 21       | 0.11          |
| (1,2609) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H  | 23       | 0.11          |
| (1,2609) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H  | 24       | 0.11          |
| (1,2609) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H  | 26       | 0.11          |
| (1,2609) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H  | 30       | 0.11          |
| (1,2609) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H  | 33       | 0.11          |
| (1,2608) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H  | 20       | 0.11          |
| (1,2608) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H  | 21       | 0.11          |
| (1,2608) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H  | 23       | 0.11          |
| (1,2608) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H  | 24       | 0.11          |
| (1,2608) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H  | 26       | 0.11          |
| (1,2608) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H  | 30       | 0.11          |
| (1,2608) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H  | 33       | 0.11          |
| (1,2550) | 1:92:A:ARG:HA  | 1:83:A:ALA:H  | 31       | 0.11          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 21       | 0.11          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 22       | 0.11          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 24       | 0.11          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 25       | 0.11          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 27       | 0.11          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 29       | 0.11          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 30       | 0.11          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 31       | 0.11          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 32       | 0.11          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 34       | 0.11          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 35       | 0.11          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 36       | 0.11          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 37       | 0.11          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 38       | 0.11          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 39       | 0.11          |
| (1,2498) | 1:9:A:PRO:HG3  | 1:9:A:PRO:HB2 | 40       | 0.11          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 26       | 0.11          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 29       | 0.11          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 33       | 0.11          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 35       | 0.11          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 36       | 0.11          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 37       | 0.11          |
| (1,2491) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HA  | 39       | 0.11          |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,2479) | 1:9:A:PRO:HD2 | 1:8:A:GLU:HA    | 3        | 0.11          |
| (1,2431) | 1:82:A:ILE:HB | 1:41:A:THR:H    | 6        | 0.11          |
| (1,2431) | 1:82:A:ILE:HB | 1:41:A:THR:H    | 7        | 0.11          |
| (1,2431) | 1:82:A:ILE:HB | 1:41:A:THR:H    | 30       | 0.11          |
| (1,2431) | 1:82:A:ILE:HB | 1:41:A:THR:H    | 31       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 1        | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 1        | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 1        | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 3        | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 3        | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 3        | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 4        | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 4        | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 4        | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 5        | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 5        | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 5        | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 6        | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 6        | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 6        | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 7        | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 7        | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 7        | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 8        | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 8        | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 8        | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 9        | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 9        | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 9        | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 10       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 10       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 10       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 12       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 12       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 12       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 13       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 13       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 13       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 14       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 14       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 14       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 15       | 0.11          |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 15       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 15       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 16       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 16       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 16       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 17       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 17       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 17       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 18       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 18       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 18       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 19       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 19       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 19       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 20       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 20       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 20       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 21       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 21       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 21       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 22       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 22       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 22       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 23       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 23       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 23       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 25       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 25       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 25       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 26       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 26       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 26       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 27       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 27       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 27       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 28       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 28       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 28       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 29       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD12 | 29       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD13 | 29       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB | 1:39:A:ILE:HD11 | 30       | 0.11          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,2424) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD12 | 30       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD13 | 30       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD11 | 31       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD12 | 31       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD13 | 31       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD11 | 32       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD12 | 32       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD13 | 32       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD11 | 33       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD12 | 33       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD13 | 33       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD11 | 34       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD12 | 34       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD13 | 34       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD11 | 35       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD12 | 35       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD13 | 35       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD11 | 37       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD12 | 37       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD13 | 37       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD11 | 39       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD12 | 39       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD13 | 39       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD11 | 40       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD12 | 40       | 0.11          |
| (1,2424) | 1:39:A:ILE:HB  | 1:39:A:ILE:HD13 | 40       | 0.11          |
| (1,2416) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 3        | 0.11          |
| (1,2416) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 4        | 0.11          |
| (1,2416) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 7        | 0.11          |
| (1,2416) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 37       | 0.11          |
| (1,2416) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 38       | 0.11          |
| (1,2416) | 1:10:A:ILE:HB  | 1:9:A:PRO:HA    | 39       | 0.11          |
| (1,2403) | 1:66:A:MET:HE1 | 1:42:A:TRP:H    | 39       | 0.11          |
| (1,2403) | 1:66:A:MET:HE2 | 1:42:A:TRP:H    | 39       | 0.11          |
| (1,2403) | 1:66:A:MET:HE3 | 1:42:A:TRP:H    | 39       | 0.11          |
| (1,2402) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ   | 6        | 0.11          |
| (1,2402) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ   | 6        | 0.11          |
| (1,2402) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ   | 6        | 0.11          |
| (1,2402) | 1:66:A:MET:HE1 | 1:29:A:PHE:HZ   | 33       | 0.11          |
| (1,2402) | 1:66:A:MET:HE2 | 1:29:A:PHE:HZ   | 33       | 0.11          |
| (1,2402) | 1:66:A:MET:HE3 | 1:29:A:PHE:HZ   | 33       | 0.11          |
| (1,2331) | 1:26:A:SER:HA  | 1:68:A:ILE:HG21 | 11       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2331) | 1:26:A:SER:HA   | 1:68:A:ILE:HG22 | 11       | 0.11          |
| (1,2331) | 1:26:A:SER:HA   | 1:68:A:ILE:HG23 | 11       | 0.11          |
| (1,2331) | 1:26:A:SER:HA   | 1:68:A:ILE:HG21 | 23       | 0.11          |
| (1,2331) | 1:26:A:SER:HA   | 1:68:A:ILE:HG22 | 23       | 0.11          |
| (1,2331) | 1:26:A:SER:HA   | 1:68:A:ILE:HG23 | 23       | 0.11          |
| (1,2331) | 1:26:A:SER:HA   | 1:68:A:ILE:HG21 | 30       | 0.11          |
| (1,2331) | 1:26:A:SER:HA   | 1:68:A:ILE:HG22 | 30       | 0.11          |
| (1,2331) | 1:26:A:SER:HA   | 1:68:A:ILE:HG23 | 30       | 0.11          |
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG21 | 26       | 0.11          |
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG22 | 26       | 0.11          |
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG23 | 26       | 0.11          |
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG21 | 39       | 0.11          |
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG22 | 39       | 0.11          |
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG23 | 39       | 0.11          |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD11 | 24       | 0.11          |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD12 | 24       | 0.11          |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD13 | 24       | 0.11          |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD11 | 32       | 0.11          |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD12 | 32       | 0.11          |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD13 | 32       | 0.11          |
| (1,2145) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 11       | 0.11          |
| (1,2145) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 25       | 0.11          |
| (1,2099) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HA   | 6        | 0.11          |
| (1,2099) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HA   | 6        | 0.11          |
| (1,2099) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HA   | 6        | 0.11          |
| (1,2099) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HA   | 20       | 0.11          |
| (1,2099) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HA   | 20       | 0.11          |
| (1,2099) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HA   | 20       | 0.11          |
| (1,2099) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HA   | 33       | 0.11          |
| (1,2099) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HA   | 33       | 0.11          |
| (1,2099) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HA   | 33       | 0.11          |
| (1,2099) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HA   | 34       | 0.11          |
| (1,2099) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HA   | 34       | 0.11          |
| (1,2099) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HA   | 34       | 0.11          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 7        | 0.11          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 7        | 0.11          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 7        | 0.11          |
| (1,2096) | 1:20:A:VAL:HG11 | 1:99:A:GLY:HA2  | 19       | 0.11          |
| (1,2096) | 1:20:A:VAL:HG12 | 1:99:A:GLY:HA2  | 19       | 0.11          |
| (1,2096) | 1:20:A:VAL:HG13 | 1:99:A:GLY:HA2  | 19       | 0.11          |
| (1,2093) | 1:88:A:ARG:HD3  | 1:7:A:ALA:HA    | 21       | 0.11          |
| (1,2087) | 1:85:A:LEU:HD11 | 1:39:A:ILE:H    | 14       | 0.11          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2087) | 1:85:A:LEU:HD12 | 1:39:A:ILE:H   | 14       | 0.11          |
| (1,2087) | 1:85:A:LEU:HD13 | 1:39:A:ILE:H   | 14       | 0.11          |
| (1,2087) | 1:85:A:LEU:HD11 | 1:39:A:ILE:H   | 17       | 0.11          |
| (1,2087) | 1:85:A:LEU:HD12 | 1:39:A:ILE:H   | 17       | 0.11          |
| (1,2087) | 1:85:A:LEU:HD13 | 1:39:A:ILE:H   | 17       | 0.11          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1 | 1        | 0.11          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2 | 1        | 0.11          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1 | 1        | 0.11          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2 | 1        | 0.11          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1 | 1        | 0.11          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2 | 1        | 0.11          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1 | 16       | 0.11          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2 | 16       | 0.11          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1 | 16       | 0.11          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2 | 16       | 0.11          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1 | 16       | 0.11          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2 | 16       | 0.11          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1 | 17       | 0.11          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2 | 17       | 0.11          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1 | 17       | 0.11          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2 | 17       | 0.11          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1 | 17       | 0.11          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2 | 17       | 0.11          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1 | 18       | 0.11          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2 | 18       | 0.11          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1 | 18       | 0.11          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2 | 18       | 0.11          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1 | 18       | 0.11          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2 | 18       | 0.11          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1 | 23       | 0.11          |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2 | 23       | 0.11          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1 | 23       | 0.11          |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2 | 23       | 0.11          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1 | 23       | 0.11          |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2 | 23       | 0.11          |
| (1,2070) | 1:97:A:LEU:HB2  | 1:19:A:ILE:HB  | 17       | 0.11          |
| (1,2070) | 1:97:A:LEU:HB2  | 1:19:A:ILE:HB  | 29       | 0.11          |
| (1,2069) | 1:94:A:THR:HG21 | 1:80:A:SER:HB3 | 28       | 0.11          |
| (1,2069) | 1:94:A:THR:HG22 | 1:80:A:SER:HB3 | 28       | 0.11          |
| (1,2069) | 1:94:A:THR:HG23 | 1:80:A:SER:HB3 | 28       | 0.11          |
| (1,2054) | 1:78:A:VAL:HG11 | 1:96:A:GLU:HG2 | 11       | 0.11          |
| (1,2054) | 1:78:A:VAL:HG12 | 1:96:A:GLU:HG2 | 11       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2054) | 1:78:A:VAL:HG13 | 1:96:A:GLU:HG2  | 11       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD21 | 27       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD22 | 27       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD23 | 27       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD21 | 27       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD22 | 27       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD23 | 27       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD21 | 27       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD22 | 27       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD23 | 27       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD21 | 29       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD22 | 29       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD23 | 29       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD21 | 29       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD22 | 29       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD23 | 29       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD21 | 29       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD22 | 29       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD23 | 29       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD21 | 36       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD22 | 36       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD23 | 36       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD21 | 36       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD22 | 36       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD23 | 36       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD21 | 36       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD22 | 36       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD23 | 36       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD21 | 39       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD22 | 39       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG21 | 1:97:A:LEU:HD23 | 39       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD21 | 39       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD22 | 39       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG22 | 1:97:A:LEU:HD23 | 39       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD21 | 39       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD22 | 39       | 0.11          |
| (1,2053) | 1:71:A:VAL:HG23 | 1:97:A:LEU:HD23 | 39       | 0.11          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1  | 7        | 0.11          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2  | 7        | 0.11          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1  | 7        | 0.11          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2  | 7        | 0.11          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1  | 7        | 0.11          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 7        | 0.11          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 28       | 0.11          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 28       | 0.11          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 28       | 0.11          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 28       | 0.11          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 28       | 0.11          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 28       | 0.11          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1 | 39       | 0.11          |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2 | 39       | 0.11          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1 | 39       | 0.11          |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2 | 39       | 0.11          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1 | 39       | 0.11          |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2 | 39       | 0.11          |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 4        | 0.11          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 4        | 0.11          |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 4        | 0.11          |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 6        | 0.11          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 6        | 0.11          |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 6        | 0.11          |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 10       | 0.11          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 10       | 0.11          |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 10       | 0.11          |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 24       | 0.11          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 24       | 0.11          |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 24       | 0.11          |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 33       | 0.11          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 33       | 0.11          |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 33       | 0.11          |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3 | 37       | 0.11          |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3 | 37       | 0.11          |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3 | 37       | 0.11          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 23       | 0.11          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 23       | 0.11          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 23       | 0.11          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 23       | 0.11          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 23       | 0.11          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 23       | 0.11          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE1 | 28       | 0.11          |
| (1,2019) | 1:49:A:LEU:HD11 | 1:57:A:PHE:HE2 | 28       | 0.11          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE1 | 28       | 0.11          |
| (1,2019) | 1:49:A:LEU:HD12 | 1:57:A:PHE:HE2 | 28       | 0.11          |
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE1 | 28       | 0.11          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2019) | 1:49:A:LEU:HD13 | 1:57:A:PHE:HE2 | 28       | 0.11          |
| (1,2014) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD1 | 1        | 0.11          |
| (1,2014) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD2 | 1        | 0.11          |
| (1,2014) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD1 | 6        | 0.11          |
| (1,2014) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD2 | 6        | 0.11          |
| (1,2014) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD1 | 12       | 0.11          |
| (1,2014) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD2 | 12       | 0.11          |
| (1,2014) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD1 | 27       | 0.11          |
| (1,2014) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD2 | 27       | 0.11          |
| (1,2014) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD1 | 39       | 0.11          |
| (1,2014) | 1:44:A:LYS:HD2  | 1:79:A:TYR:HD2 | 39       | 0.11          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1 | 2        | 0.11          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2 | 2        | 0.11          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3 | 2        | 0.11          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1 | 2        | 0.11          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2 | 2        | 0.11          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3 | 2        | 0.11          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1 | 2        | 0.11          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2 | 2        | 0.11          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3 | 2        | 0.11          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1 | 13       | 0.11          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2 | 13       | 0.11          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3 | 13       | 0.11          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1 | 13       | 0.11          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2 | 13       | 0.11          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3 | 13       | 0.11          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1 | 13       | 0.11          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2 | 13       | 0.11          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3 | 13       | 0.11          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1 | 14       | 0.11          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2 | 14       | 0.11          |
| (1,2010) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3 | 14       | 0.11          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1 | 14       | 0.11          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2 | 14       | 0.11          |
| (1,2010) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3 | 14       | 0.11          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1 | 14       | 0.11          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2 | 14       | 0.11          |
| (1,2010) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3 | 14       | 0.11          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 12       | 0.11          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 29       | 0.11          |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H   | 38       | 0.11          |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2 | 19       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 19       | 0.11          |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 19       | 0.11          |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 23       | 0.11          |
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 23       | 0.11          |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 23       | 0.11          |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 24       | 0.11          |
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 24       | 0.11          |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 24       | 0.11          |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 33       | 0.11          |
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 33       | 0.11          |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 33       | 0.11          |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 38       | 0.11          |
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 38       | 0.11          |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 38       | 0.11          |
| (1,1994) | 1:21:A:VAL:HG11 | 1:25:A:GLN:HG3  | 8        | 0.11          |
| (1,1994) | 1:21:A:VAL:HG12 | 1:25:A:GLN:HG3  | 8        | 0.11          |
| (1,1994) | 1:21:A:VAL:HG13 | 1:25:A:GLN:HG3  | 8        | 0.11          |
| (1,1994) | 1:21:A:VAL:HG11 | 1:25:A:GLN:HG3  | 16       | 0.11          |
| (1,1994) | 1:21:A:VAL:HG12 | 1:25:A:GLN:HG3  | 16       | 0.11          |
| (1,1994) | 1:21:A:VAL:HG13 | 1:25:A:GLN:HG3  | 16       | 0.11          |
| (1,1994) | 1:21:A:VAL:HG11 | 1:25:A:GLN:HG3  | 33       | 0.11          |
| (1,1994) | 1:21:A:VAL:HG12 | 1:25:A:GLN:HG3  | 33       | 0.11          |
| (1,1994) | 1:21:A:VAL:HG13 | 1:25:A:GLN:HG3  | 33       | 0.11          |
| (1,1994) | 1:21:A:VAL:HG11 | 1:25:A:GLN:HG3  | 38       | 0.11          |
| (1,1994) | 1:21:A:VAL:HG12 | 1:25:A:GLN:HG3  | 38       | 0.11          |
| (1,1994) | 1:21:A:VAL:HG13 | 1:25:A:GLN:HG3  | 38       | 0.11          |
| (1,1990) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 10       | 0.11          |
| (1,1990) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 10       | 0.11          |
| (1,1990) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 10       | 0.11          |
| (1,1990) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 13       | 0.11          |
| (1,1990) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 13       | 0.11          |
| (1,1990) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 13       | 0.11          |
| (1,1990) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 31       | 0.11          |
| (1,1990) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 31       | 0.11          |
| (1,1990) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 31       | 0.11          |
| (1,1990) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 32       | 0.11          |
| (1,1990) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 32       | 0.11          |
| (1,1990) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 32       | 0.11          |
| (1,1990) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 37       | 0.11          |
| (1,1990) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 37       | 0.11          |
| (1,1990) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 37       | 0.11          |
| (1,1990) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 39       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1990) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 39       | 0.11          |
| (1,1990) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 39       | 0.11          |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 18       | 0.11          |
| (1,1956) | 1:72:A:THR:HG21 | 1:74:A:ASP:HB3  | 7        | 0.11          |
| (1,1956) | 1:72:A:THR:HG22 | 1:74:A:ASP:HB3  | 7        | 0.11          |
| (1,1956) | 1:72:A:THR:HG23 | 1:74:A:ASP:HB3  | 7        | 0.11          |
| (1,1956) | 1:72:A:THR:HG21 | 1:74:A:ASP:HB3  | 31       | 0.11          |
| (1,1956) | 1:72:A:THR:HG22 | 1:74:A:ASP:HB3  | 31       | 0.11          |
| (1,1956) | 1:72:A:THR:HG23 | 1:74:A:ASP:HB3  | 31       | 0.11          |
| (1,1952) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB1  | 9        | 0.11          |
| (1,1952) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB2  | 9        | 0.11          |
| (1,1952) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB3  | 9        | 0.11          |
| (1,1952) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB1  | 9        | 0.11          |
| (1,1952) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB2  | 9        | 0.11          |
| (1,1952) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB3  | 9        | 0.11          |
| (1,1952) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB1  | 9        | 0.11          |
| (1,1952) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB2  | 9        | 0.11          |
| (1,1952) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB3  | 9        | 0.11          |
| (1,1952) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB1  | 17       | 0.11          |
| (1,1952) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB2  | 17       | 0.11          |
| (1,1952) | 1:68:A:ILE:HD11 | 1:27:A:ALA:HB3  | 17       | 0.11          |
| (1,1952) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB1  | 17       | 0.11          |
| (1,1952) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB2  | 17       | 0.11          |
| (1,1952) | 1:68:A:ILE:HD12 | 1:27:A:ALA:HB3  | 17       | 0.11          |
| (1,1952) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB1  | 17       | 0.11          |
| (1,1952) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB2  | 17       | 0.11          |
| (1,1952) | 1:68:A:ILE:HD13 | 1:27:A:ALA:HB3  | 17       | 0.11          |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H    | 1        | 0.11          |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H    | 1        | 0.11          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H    | 1        | 0.11          |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H    | 2        | 0.11          |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H    | 2        | 0.11          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H    | 2        | 0.11          |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H    | 5        | 0.11          |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H    | 5        | 0.11          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H    | 5        | 0.11          |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H    | 9        | 0.11          |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H    | 9        | 0.11          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H    | 9        | 0.11          |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H    | 15       | 0.11          |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H    | 15       | 0.11          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H    | 15       | 0.11          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 17       | 0.11          |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 17       | 0.11          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 17       | 0.11          |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 26       | 0.11          |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 26       | 0.11          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 26       | 0.11          |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 28       | 0.11          |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 28       | 0.11          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 28       | 0.11          |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H   | 29       | 0.11          |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H   | 29       | 0.11          |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H   | 29       | 0.11          |
| (1,1907) | 1:68:A:ILE:HG21 | 1:54:A:LYS:HD2 | 28       | 0.11          |
| (1,1907) | 1:68:A:ILE:HG22 | 1:54:A:LYS:HD2 | 28       | 0.11          |
| (1,1907) | 1:68:A:ILE:HG23 | 1:54:A:LYS:HD2 | 28       | 0.11          |
| (1,1903) | 1:66:A:MET:HE1  | 1:79:A:TYR:HA  | 16       | 0.11          |
| (1,1903) | 1:66:A:MET:HE2  | 1:79:A:TYR:HA  | 16       | 0.11          |
| (1,1903) | 1:66:A:MET:HE3  | 1:79:A:TYR:HA  | 16       | 0.11          |
| (1,1903) | 1:66:A:MET:HE1  | 1:79:A:TYR:HA  | 21       | 0.11          |
| (1,1903) | 1:66:A:MET:HE2  | 1:79:A:TYR:HA  | 21       | 0.11          |
| (1,1903) | 1:66:A:MET:HE3  | 1:79:A:TYR:HA  | 21       | 0.11          |
| (1,1901) | 1:49:A:LEU:HD21 | 1:44:A:LYS:HG2 | 2        | 0.11          |
| (1,1901) | 1:49:A:LEU:HD22 | 1:44:A:LYS:HG2 | 2        | 0.11          |
| (1,1901) | 1:49:A:LEU:HD23 | 1:44:A:LYS:HG2 | 2        | 0.11          |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 7        | 0.11          |
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 7        | 0.11          |
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 7        | 0.11          |
| (1,1899) | 1:49:A:LEU:HD11 | 1:43:A:TYR:HA  | 11       | 0.11          |
| (1,1899) | 1:49:A:LEU:HD12 | 1:43:A:TYR:HA  | 11       | 0.11          |
| (1,1899) | 1:49:A:LEU:HD13 | 1:43:A:TYR:HA  | 11       | 0.11          |
| (1,1896) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3 | 2        | 0.11          |
| (1,1896) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3 | 2        | 0.11          |
| (1,1896) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3 | 2        | 0.11          |
| (1,1896) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3 | 12       | 0.11          |
| (1,1896) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3 | 12       | 0.11          |
| (1,1896) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3 | 12       | 0.11          |
| (1,1861) | 1:7:A:ALA:HB1   | 1:88:A:ARG:HA  | 1        | 0.11          |
| (1,1861) | 1:7:A:ALA:HB2   | 1:88:A:ARG:HA  | 1        | 0.11          |
| (1,1861) | 1:7:A:ALA:HB3   | 1:88:A:ARG:HA  | 1        | 0.11          |
| (1,1861) | 1:7:A:ALA:HB1   | 1:88:A:ARG:HA  | 36       | 0.11          |
| (1,1861) | 1:7:A:ALA:HB2   | 1:88:A:ARG:HA  | 36       | 0.11          |
| (1,1861) | 1:7:A:ALA:HB3   | 1:88:A:ARG:HA  | 36       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1861) | 1:7:A:ALA:HB1   | 1:88:A:ARG:HA   | 39       | 0.11          |
| (1,1861) | 1:7:A:ALA:HB2   | 1:88:A:ARG:HA   | 39       | 0.11          |
| (1,1861) | 1:7:A:ALA:HB3   | 1:88:A:ARG:HA   | 39       | 0.11          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG11 | 22       | 0.11          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG12 | 22       | 0.11          |
| (1,1717) | 1:38:A:ALA:HB1  | 1:33:A:VAL:HG13 | 22       | 0.11          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG11 | 22       | 0.11          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG12 | 22       | 0.11          |
| (1,1717) | 1:38:A:ALA:HB2  | 1:33:A:VAL:HG13 | 22       | 0.11          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG11 | 22       | 0.11          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG12 | 22       | 0.11          |
| (1,1717) | 1:38:A:ALA:HB3  | 1:33:A:VAL:HG13 | 22       | 0.11          |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 6        | 0.11          |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 6        | 0.11          |
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 6        | 0.11          |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 7        | 0.11          |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 7        | 0.11          |
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 7        | 0.11          |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 8        | 0.11          |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 8        | 0.11          |
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 8        | 0.11          |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 21       | 0.11          |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 21       | 0.11          |
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 21       | 0.11          |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 23       | 0.11          |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 23       | 0.11          |
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 23       | 0.11          |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 30       | 0.11          |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 30       | 0.11          |
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 30       | 0.11          |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 32       | 0.11          |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 32       | 0.11          |
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 32       | 0.11          |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 33       | 0.11          |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 33       | 0.11          |
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 33       | 0.11          |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 34       | 0.11          |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 34       | 0.11          |
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 34       | 0.11          |
| (1,1708) | 1:49:A:LEU:HD21 | 1:49:A:LEU:H    | 35       | 0.11          |
| (1,1708) | 1:49:A:LEU:HD22 | 1:49:A:LEU:H    | 35       | 0.11          |
| (1,1708) | 1:49:A:LEU:HD23 | 1:49:A:LEU:H    | 35       | 0.11          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1708) | 1:49:A:LEU:HD21  | 1:49:A:LEU:H    | 39       | 0.11          |
| (1,1708) | 1:49:A:LEU:HD22  | 1:49:A:LEU:H    | 39       | 0.11          |
| (1,1708) | 1:49:A:LEU:HD23  | 1:49:A:LEU:H    | 39       | 0.11          |
| (1,1708) | 1:49:A:LEU:HD21  | 1:49:A:LEU:H    | 40       | 0.11          |
| (1,1708) | 1:49:A:LEU:HD22  | 1:49:A:LEU:H    | 40       | 0.11          |
| (1,1708) | 1:49:A:LEU:HD23  | 1:49:A:LEU:H    | 40       | 0.11          |
| (1,1706) | 1:49:A:LEU:HD21  | 1:50:A:THR:H    | 35       | 0.11          |
| (1,1706) | 1:49:A:LEU:HD22  | 1:50:A:THR:H    | 35       | 0.11          |
| (1,1706) | 1:49:A:LEU:HD23  | 1:50:A:THR:H    | 35       | 0.11          |
| (1,1696) | 1:101:A:LEU:HD21 | 1:101:A:LEU:HB3 | 31       | 0.11          |
| (1,1696) | 1:101:A:LEU:HD22 | 1:101:A:LEU:HB3 | 31       | 0.11          |
| (1,1696) | 1:101:A:LEU:HD23 | 1:101:A:LEU:HB3 | 31       | 0.11          |
| (1,1685) | 1:97:A:LEU:HD11  | 1:71:A:VAL:HG21 | 6        | 0.11          |
| (1,1685) | 1:97:A:LEU:HD11  | 1:71:A:VAL:HG22 | 6        | 0.11          |
| (1,1685) | 1:97:A:LEU:HD11  | 1:71:A:VAL:HG23 | 6        | 0.11          |
| (1,1685) | 1:97:A:LEU:HD12  | 1:71:A:VAL:HG21 | 6        | 0.11          |
| (1,1685) | 1:97:A:LEU:HD12  | 1:71:A:VAL:HG22 | 6        | 0.11          |
| (1,1685) | 1:97:A:LEU:HD12  | 1:71:A:VAL:HG23 | 6        | 0.11          |
| (1,1685) | 1:97:A:LEU:HD13  | 1:71:A:VAL:HG21 | 6        | 0.11          |
| (1,1685) | 1:97:A:LEU:HD13  | 1:71:A:VAL:HG22 | 6        | 0.11          |
| (1,1685) | 1:97:A:LEU:HD13  | 1:71:A:VAL:HG23 | 6        | 0.11          |
| (1,1685) | 1:97:A:LEU:HD11  | 1:71:A:VAL:HG21 | 7        | 0.11          |
| (1,1685) | 1:97:A:LEU:HD11  | 1:71:A:VAL:HG22 | 7        | 0.11          |
| (1,1685) | 1:97:A:LEU:HD11  | 1:71:A:VAL:HG23 | 7        | 0.11          |
| (1,1685) | 1:97:A:LEU:HD12  | 1:71:A:VAL:HG21 | 7        | 0.11          |
| (1,1685) | 1:97:A:LEU:HD12  | 1:71:A:VAL:HG22 | 7        | 0.11          |
| (1,1685) | 1:97:A:LEU:HD12  | 1:71:A:VAL:HG23 | 7        | 0.11          |
| (1,1685) | 1:97:A:LEU:HD13  | 1:71:A:VAL:HG21 | 7        | 0.11          |
| (1,1685) | 1:97:A:LEU:HD13  | 1:71:A:VAL:HG22 | 7        | 0.11          |
| (1,1685) | 1:97:A:LEU:HD13  | 1:71:A:VAL:HG23 | 7        | 0.11          |
| (1,1685) | 1:97:A:LEU:HD11  | 1:71:A:VAL:HG21 | 23       | 0.11          |
| (1,1685) | 1:97:A:LEU:HD11  | 1:71:A:VAL:HG22 | 23       | 0.11          |
| (1,1685) | 1:97:A:LEU:HD11  | 1:71:A:VAL:HG23 | 23       | 0.11          |
| (1,1685) | 1:97:A:LEU:HD12  | 1:71:A:VAL:HG21 | 23       | 0.11          |
| (1,1685) | 1:97:A:LEU:HD12  | 1:71:A:VAL:HG22 | 23       | 0.11          |
| (1,1685) | 1:97:A:LEU:HD12  | 1:71:A:VAL:HG23 | 23       | 0.11          |
| (1,1685) | 1:97:A:LEU:HD13  | 1:71:A:VAL:HG21 | 23       | 0.11          |
| (1,1685) | 1:97:A:LEU:HD13  | 1:71:A:VAL:HG22 | 23       | 0.11          |
| (1,1685) | 1:97:A:LEU:HD13  | 1:71:A:VAL:HG23 | 23       | 0.11          |
| (1,1678) | 1:85:A:LEU:HD11  | 1:85:A:LEU:HA   | 30       | 0.11          |
| (1,1678) | 1:85:A:LEU:HD12  | 1:85:A:LEU:HA   | 30       | 0.11          |
| (1,1678) | 1:85:A:LEU:HD13  | 1:85:A:LEU:HA   | 30       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 39       | 0.11          |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 39       | 0.11          |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 39       | 0.11          |
| (1,1654) | 1:40:A:VAL:HB   | 1:39:A:ILE:HA   | 2        | 0.11          |
| (1,1654) | 1:40:A:VAL:HB   | 1:39:A:ILE:HA   | 24       | 0.11          |
| (1,1654) | 1:40:A:VAL:HB   | 1:39:A:ILE:HA   | 36       | 0.11          |
| (1,1650) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 4        | 0.11          |
| (1,1650) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 4        | 0.11          |
| (1,1650) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 4        | 0.11          |
| (1,1650) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 4        | 0.11          |
| (1,1650) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 4        | 0.11          |
| (1,1650) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 4        | 0.11          |
| (1,1650) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 4        | 0.11          |
| (1,1650) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 4        | 0.11          |
| (1,1650) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 4        | 0.11          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 15       | 0.11          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 15       | 0.11          |
| (1,1639) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 15       | 0.11          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 15       | 0.11          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 15       | 0.11          |
| (1,1639) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 15       | 0.11          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 15       | 0.11          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 15       | 0.11          |
| (1,1639) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 15       | 0.11          |
| (1,1624) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2  | 17       | 0.11          |
| (1,1624) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2  | 17       | 0.11          |
| (1,1624) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2  | 17       | 0.11          |
| (1,1624) | 1:82:A:ILE:HG21 | 1:90:A:GLU:HG2  | 31       | 0.11          |
| (1,1624) | 1:82:A:ILE:HG22 | 1:90:A:GLU:HG2  | 31       | 0.11          |
| (1,1624) | 1:82:A:ILE:HG23 | 1:90:A:GLU:HG2  | 31       | 0.11          |
| (1,1623) | 1:82:A:ILE:HG21 | 1:84:A:ARG:HG2  | 20       | 0.11          |
| (1,1623) | 1:82:A:ILE:HG22 | 1:84:A:ARG:HG2  | 20       | 0.11          |
| (1,1623) | 1:82:A:ILE:HG23 | 1:84:A:ARG:HG2  | 20       | 0.11          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1  | 6        | 0.11          |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2  | 6        | 0.11          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1  | 6        | 0.11          |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2  | 6        | 0.11          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1  | 6        | 0.11          |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2  | 6        | 0.11          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 3        | 0.11          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 3        | 0.11          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 3        | 0.11          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 3        | 0.11          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 3        | 0.11          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 3        | 0.11          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 6        | 0.11          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 6        | 0.11          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 6        | 0.11          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 6        | 0.11          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 6        | 0.11          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 6        | 0.11          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1 | 29       | 0.11          |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2 | 29       | 0.11          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1 | 29       | 0.11          |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2 | 29       | 0.11          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1 | 29       | 0.11          |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2 | 29       | 0.11          |
| (1,1550) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA   | 21       | 0.11          |
| (1,1550) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA   | 21       | 0.11          |
| (1,1550) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA   | 21       | 0.11          |
| (1,1550) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA   | 24       | 0.11          |
| (1,1550) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA   | 24       | 0.11          |
| (1,1550) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA   | 24       | 0.11          |
| (1,1550) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA   | 25       | 0.11          |
| (1,1550) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA   | 25       | 0.11          |
| (1,1550) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA   | 25       | 0.11          |
| (1,1550) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA   | 32       | 0.11          |
| (1,1550) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA   | 32       | 0.11          |
| (1,1550) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA   | 32       | 0.11          |
| (1,1550) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA   | 37       | 0.11          |
| (1,1550) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA   | 37       | 0.11          |
| (1,1550) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA   | 37       | 0.11          |
| (1,1550) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA   | 38       | 0.11          |
| (1,1550) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA   | 38       | 0.11          |
| (1,1550) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA   | 38       | 0.11          |
| (1,1548) | 1:10:A:ILE:HG21 | 1:83:A:ALA:HB1 | 3        | 0.11          |
| (1,1548) | 1:10:A:ILE:HG21 | 1:83:A:ALA:HB2 | 3        | 0.11          |
| (1,1548) | 1:10:A:ILE:HG21 | 1:83:A:ALA:HB3 | 3        | 0.11          |
| (1,1548) | 1:10:A:ILE:HG22 | 1:83:A:ALA:HB1 | 3        | 0.11          |
| (1,1548) | 1:10:A:ILE:HG22 | 1:83:A:ALA:HB2 | 3        | 0.11          |
| (1,1548) | 1:10:A:ILE:HG22 | 1:83:A:ALA:HB3 | 3        | 0.11          |
| (1,1548) | 1:10:A:ILE:HG23 | 1:83:A:ALA:HB1 | 3        | 0.11          |
| (1,1548) | 1:10:A:ILE:HG23 | 1:83:A:ALA:HB2 | 3        | 0.11          |
| (1,1548) | 1:10:A:ILE:HG23 | 1:83:A:ALA:HB3 | 3        | 0.11          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1548) | 1:10:A:ILE:HG21 | 1:83:A:ALA:HB1 | 10       | 0.11          |
| (1,1548) | 1:10:A:ILE:HG21 | 1:83:A:ALA:HB2 | 10       | 0.11          |
| (1,1548) | 1:10:A:ILE:HG21 | 1:83:A:ALA:HB3 | 10       | 0.11          |
| (1,1548) | 1:10:A:ILE:HG22 | 1:83:A:ALA:HB1 | 10       | 0.11          |
| (1,1548) | 1:10:A:ILE:HG22 | 1:83:A:ALA:HB2 | 10       | 0.11          |
| (1,1548) | 1:10:A:ILE:HG22 | 1:83:A:ALA:HB3 | 10       | 0.11          |
| (1,1548) | 1:10:A:ILE:HG23 | 1:83:A:ALA:HB1 | 10       | 0.11          |
| (1,1548) | 1:10:A:ILE:HG23 | 1:83:A:ALA:HB2 | 10       | 0.11          |
| (1,1548) | 1:10:A:ILE:HG23 | 1:83:A:ALA:HB3 | 10       | 0.11          |
| (1,1548) | 1:10:A:ILE:HG21 | 1:83:A:ALA:HB1 | 14       | 0.11          |
| (1,1548) | 1:10:A:ILE:HG21 | 1:83:A:ALA:HB2 | 14       | 0.11          |
| (1,1548) | 1:10:A:ILE:HG21 | 1:83:A:ALA:HB3 | 14       | 0.11          |
| (1,1548) | 1:10:A:ILE:HG22 | 1:83:A:ALA:HB1 | 14       | 0.11          |
| (1,1548) | 1:10:A:ILE:HG22 | 1:83:A:ALA:HB2 | 14       | 0.11          |
| (1,1548) | 1:10:A:ILE:HG22 | 1:83:A:ALA:HB3 | 14       | 0.11          |
| (1,1548) | 1:10:A:ILE:HG23 | 1:83:A:ALA:HB1 | 14       | 0.11          |
| (1,1548) | 1:10:A:ILE:HG23 | 1:83:A:ALA:HB2 | 14       | 0.11          |
| (1,1548) | 1:10:A:ILE:HG23 | 1:83:A:ALA:HB3 | 14       | 0.11          |
| (1,1518) | 1:66:A:MET:HE1  | 1:66:A:MET:HA  | 6        | 0.11          |
| (1,1518) | 1:66:A:MET:HE2  | 1:66:A:MET:HA  | 6        | 0.11          |
| (1,1518) | 1:66:A:MET:HE3  | 1:66:A:MET:HA  | 6        | 0.11          |
| (1,1513) | 1:66:A:MET:HE1  | 1:29:A:PHE:H   | 9        | 0.11          |
| (1,1513) | 1:66:A:MET:HE2  | 1:29:A:PHE:H   | 9        | 0.11          |
| (1,1513) | 1:66:A:MET:HE3  | 1:29:A:PHE:H   | 9        | 0.11          |
| (1,1513) | 1:66:A:MET:HE1  | 1:29:A:PHE:H   | 14       | 0.11          |
| (1,1513) | 1:66:A:MET:HE2  | 1:29:A:PHE:H   | 14       | 0.11          |
| (1,1513) | 1:66:A:MET:HE3  | 1:29:A:PHE:H   | 14       | 0.11          |
| (1,1513) | 1:66:A:MET:HE1  | 1:29:A:PHE:H   | 22       | 0.11          |
| (1,1513) | 1:66:A:MET:HE2  | 1:29:A:PHE:H   | 22       | 0.11          |
| (1,1513) | 1:66:A:MET:HE3  | 1:29:A:PHE:H   | 22       | 0.11          |
| (1,1513) | 1:66:A:MET:HE1  | 1:29:A:PHE:H   | 25       | 0.11          |
| (1,1513) | 1:66:A:MET:HE2  | 1:29:A:PHE:H   | 25       | 0.11          |
| (1,1513) | 1:66:A:MET:HE3  | 1:29:A:PHE:H   | 25       | 0.11          |
| (1,1513) | 1:66:A:MET:HE1  | 1:29:A:PHE:H   | 30       | 0.11          |
| (1,1513) | 1:66:A:MET:HE2  | 1:29:A:PHE:H   | 30       | 0.11          |
| (1,1513) | 1:66:A:MET:HE3  | 1:29:A:PHE:H   | 30       | 0.11          |
| (1,1510) | 1:66:A:MET:HE1  | 1:42:A:TRP:HE1 | 2        | 0.11          |
| (1,1510) | 1:66:A:MET:HE2  | 1:42:A:TRP:HE1 | 2        | 0.11          |
| (1,1510) | 1:66:A:MET:HE3  | 1:42:A:TRP:HE1 | 2        | 0.11          |
| (1,1510) | 1:66:A:MET:HE1  | 1:42:A:TRP:HE1 | 4        | 0.11          |
| (1,1510) | 1:66:A:MET:HE2  | 1:42:A:TRP:HE1 | 4        | 0.11          |
| (1,1510) | 1:66:A:MET:HE3  | 1:42:A:TRP:HE1 | 4        | 0.11          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1510) | 1:66:A:MET:HE1 | 1:42:A:TRP:HE1 | 14       | 0.11          |
| (1,1510) | 1:66:A:MET:HE2 | 1:42:A:TRP:HE1 | 14       | 0.11          |
| (1,1510) | 1:66:A:MET:HE3 | 1:42:A:TRP:HE1 | 14       | 0.11          |
| (1,1510) | 1:66:A:MET:HE1 | 1:42:A:TRP:HE1 | 23       | 0.11          |
| (1,1510) | 1:66:A:MET:HE2 | 1:42:A:TRP:HE1 | 23       | 0.11          |
| (1,1510) | 1:66:A:MET:HE3 | 1:42:A:TRP:HE1 | 23       | 0.11          |
| (1,1510) | 1:66:A:MET:HE1 | 1:42:A:TRP:HE1 | 24       | 0.11          |
| (1,1510) | 1:66:A:MET:HE2 | 1:42:A:TRP:HE1 | 24       | 0.11          |
| (1,1510) | 1:66:A:MET:HE3 | 1:42:A:TRP:HE1 | 24       | 0.11          |
| (1,1510) | 1:66:A:MET:HE1 | 1:42:A:TRP:HE1 | 32       | 0.11          |
| (1,1510) | 1:66:A:MET:HE2 | 1:42:A:TRP:HE1 | 32       | 0.11          |
| (1,1510) | 1:66:A:MET:HE3 | 1:42:A:TRP:HE1 | 32       | 0.11          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE1 | 39       | 0.11          |
| (1,1509) | 1:66:A:MET:HE1 | 1:79:A:TYR:HE2 | 39       | 0.11          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE1 | 39       | 0.11          |
| (1,1509) | 1:66:A:MET:HE2 | 1:79:A:TYR:HE2 | 39       | 0.11          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE1 | 39       | 0.11          |
| (1,1509) | 1:66:A:MET:HE3 | 1:79:A:TYR:HE2 | 39       | 0.11          |
| (1,1507) | 1:66:A:MET:HE1 | 1:42:A:TRP:HB2 | 3        | 0.11          |
| (1,1507) | 1:66:A:MET:HE2 | 1:42:A:TRP:HB2 | 3        | 0.11          |
| (1,1507) | 1:66:A:MET:HE3 | 1:42:A:TRP:HB2 | 3        | 0.11          |
| (1,1507) | 1:66:A:MET:HE1 | 1:42:A:TRP:HB2 | 9        | 0.11          |
| (1,1507) | 1:66:A:MET:HE2 | 1:42:A:TRP:HB2 | 9        | 0.11          |
| (1,1507) | 1:66:A:MET:HE3 | 1:42:A:TRP:HB2 | 9        | 0.11          |
| (1,1507) | 1:66:A:MET:HE1 | 1:42:A:TRP:HB2 | 11       | 0.11          |
| (1,1507) | 1:66:A:MET:HE2 | 1:42:A:TRP:HB2 | 11       | 0.11          |
| (1,1507) | 1:66:A:MET:HE3 | 1:42:A:TRP:HB2 | 11       | 0.11          |
| (1,1507) | 1:66:A:MET:HE1 | 1:42:A:TRP:HB2 | 18       | 0.11          |
| (1,1507) | 1:66:A:MET:HE2 | 1:42:A:TRP:HB2 | 18       | 0.11          |
| (1,1507) | 1:66:A:MET:HE3 | 1:42:A:TRP:HB2 | 18       | 0.11          |
| (1,1507) | 1:66:A:MET:HE1 | 1:42:A:TRP:HB2 | 20       | 0.11          |
| (1,1507) | 1:66:A:MET:HE2 | 1:42:A:TRP:HB2 | 20       | 0.11          |
| (1,1507) | 1:66:A:MET:HE3 | 1:42:A:TRP:HB2 | 20       | 0.11          |
| (1,1507) | 1:66:A:MET:HE1 | 1:42:A:TRP:HB2 | 23       | 0.11          |
| (1,1507) | 1:66:A:MET:HE2 | 1:42:A:TRP:HB2 | 23       | 0.11          |
| (1,1507) | 1:66:A:MET:HE3 | 1:42:A:TRP:HB2 | 23       | 0.11          |
| (1,1507) | 1:66:A:MET:HE1 | 1:42:A:TRP:HB2 | 25       | 0.11          |
| (1,1507) | 1:66:A:MET:HE2 | 1:42:A:TRP:HB2 | 25       | 0.11          |
| (1,1507) | 1:66:A:MET:HE3 | 1:42:A:TRP:HB2 | 25       | 0.11          |
| (1,1507) | 1:66:A:MET:HE1 | 1:42:A:TRP:HB2 | 26       | 0.11          |
| (1,1507) | 1:66:A:MET:HE2 | 1:42:A:TRP:HB2 | 26       | 0.11          |
| (1,1507) | 1:66:A:MET:HE3 | 1:42:A:TRP:HB2 | 26       | 0.11          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1507) | 1:66:A:MET:HE1 | 1:42:A:TRP:HB2  | 30       | 0.11          |
| (1,1507) | 1:66:A:MET:HE2 | 1:42:A:TRP:HB2  | 30       | 0.11          |
| (1,1507) | 1:66:A:MET:HE3 | 1:42:A:TRP:HB2  | 30       | 0.11          |
| (1,1507) | 1:66:A:MET:HE1 | 1:42:A:TRP:HB2  | 31       | 0.11          |
| (1,1507) | 1:66:A:MET:HE2 | 1:42:A:TRP:HB2  | 31       | 0.11          |
| (1,1507) | 1:66:A:MET:HE3 | 1:42:A:TRP:HB2  | 31       | 0.11          |
| (1,1503) | 1:66:A:MET:HE1 | 1:66:A:MET:HG2  | 4        | 0.11          |
| (1,1503) | 1:66:A:MET:HE2 | 1:66:A:MET:HG2  | 4        | 0.11          |
| (1,1503) | 1:66:A:MET:HE3 | 1:66:A:MET:HG2  | 4        | 0.11          |
| (1,1503) | 1:66:A:MET:HE1 | 1:66:A:MET:HG2  | 15       | 0.11          |
| (1,1503) | 1:66:A:MET:HE2 | 1:66:A:MET:HG2  | 15       | 0.11          |
| (1,1503) | 1:66:A:MET:HE3 | 1:66:A:MET:HG2  | 15       | 0.11          |
| (1,1503) | 1:66:A:MET:HE1 | 1:66:A:MET:HG2  | 16       | 0.11          |
| (1,1503) | 1:66:A:MET:HE2 | 1:66:A:MET:HG2  | 16       | 0.11          |
| (1,1503) | 1:66:A:MET:HE3 | 1:66:A:MET:HG2  | 16       | 0.11          |
| (1,1503) | 1:66:A:MET:HE1 | 1:66:A:MET:HG2  | 19       | 0.11          |
| (1,1503) | 1:66:A:MET:HE2 | 1:66:A:MET:HG2  | 19       | 0.11          |
| (1,1503) | 1:66:A:MET:HE3 | 1:66:A:MET:HG2  | 19       | 0.11          |
| (1,1503) | 1:66:A:MET:HE1 | 1:66:A:MET:HG2  | 29       | 0.11          |
| (1,1503) | 1:66:A:MET:HE2 | 1:66:A:MET:HG2  | 29       | 0.11          |
| (1,1503) | 1:66:A:MET:HE3 | 1:66:A:MET:HG2  | 29       | 0.11          |
| (1,1503) | 1:66:A:MET:HE1 | 1:66:A:MET:HG2  | 33       | 0.11          |
| (1,1503) | 1:66:A:MET:HE2 | 1:66:A:MET:HG2  | 33       | 0.11          |
| (1,1503) | 1:66:A:MET:HE3 | 1:66:A:MET:HG2  | 33       | 0.11          |
| (1,1503) | 1:66:A:MET:HE1 | 1:66:A:MET:HG2  | 39       | 0.11          |
| (1,1503) | 1:66:A:MET:HE2 | 1:66:A:MET:HG2  | 39       | 0.11          |
| (1,1503) | 1:66:A:MET:HE3 | 1:66:A:MET:HG2  | 39       | 0.11          |
| (1,1502) | 1:66:A:MET:HE1 | 1:49:A:LEU:HD11 | 9        | 0.11          |
| (1,1502) | 1:66:A:MET:HE1 | 1:49:A:LEU:HD12 | 9        | 0.11          |
| (1,1502) | 1:66:A:MET:HE1 | 1:49:A:LEU:HD13 | 9        | 0.11          |
| (1,1502) | 1:66:A:MET:HE2 | 1:49:A:LEU:HD11 | 9        | 0.11          |
| (1,1502) | 1:66:A:MET:HE2 | 1:49:A:LEU:HD12 | 9        | 0.11          |
| (1,1502) | 1:66:A:MET:HE2 | 1:49:A:LEU:HD13 | 9        | 0.11          |
| (1,1502) | 1:66:A:MET:HE3 | 1:49:A:LEU:HD11 | 9        | 0.11          |
| (1,1502) | 1:66:A:MET:HE3 | 1:49:A:LEU:HD12 | 9        | 0.11          |
| (1,1502) | 1:66:A:MET:HE3 | 1:49:A:LEU:HD13 | 9        | 0.11          |
| (1,1502) | 1:66:A:MET:HE1 | 1:49:A:LEU:HD11 | 35       | 0.11          |
| (1,1502) | 1:66:A:MET:HE1 | 1:49:A:LEU:HD12 | 35       | 0.11          |
| (1,1502) | 1:66:A:MET:HE1 | 1:49:A:LEU:HD13 | 35       | 0.11          |
| (1,1502) | 1:66:A:MET:HE2 | 1:49:A:LEU:HD11 | 35       | 0.11          |
| (1,1502) | 1:66:A:MET:HE2 | 1:49:A:LEU:HD12 | 35       | 0.11          |
| (1,1502) | 1:66:A:MET:HE2 | 1:49:A:LEU:HD13 | 35       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1502) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD11 | 35       | 0.11          |
| (1,1502) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD12 | 35       | 0.11          |
| (1,1502) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD13 | 35       | 0.11          |
| (1,1494) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 12       | 0.11          |
| (1,1494) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 12       | 0.11          |
| (1,1494) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 12       | 0.11          |
| (1,1494) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 15       | 0.11          |
| (1,1494) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 15       | 0.11          |
| (1,1494) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 15       | 0.11          |
| (1,1494) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 23       | 0.11          |
| (1,1494) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 23       | 0.11          |
| (1,1494) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 23       | 0.11          |
| (1,1494) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 33       | 0.11          |
| (1,1494) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 33       | 0.11          |
| (1,1494) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 33       | 0.11          |
| (1,1494) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 39       | 0.11          |
| (1,1494) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 39       | 0.11          |
| (1,1494) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 39       | 0.11          |
| (1,1484) | 1:81:A:VAL:HB   | 1:42:A:TRP:HE1  | 10       | 0.11          |
| (1,1484) | 1:81:A:VAL:HB   | 1:42:A:TRP:HE1  | 11       | 0.11          |
| (1,1484) | 1:81:A:VAL:HB   | 1:42:A:TRP:HE1  | 34       | 0.11          |
| (1,1436) | 1:33:A:VAL:HG21 | 1:32:A:GLU:HA   | 27       | 0.11          |
| (1,1436) | 1:33:A:VAL:HG22 | 1:32:A:GLU:HA   | 27       | 0.11          |
| (1,1436) | 1:33:A:VAL:HG23 | 1:32:A:GLU:HA   | 27       | 0.11          |
| (1,1420) | 1:21:A:VAL:HG21 | 1:19:A:ILE:HD11 | 9        | 0.11          |
| (1,1420) | 1:21:A:VAL:HG21 | 1:19:A:ILE:HD12 | 9        | 0.11          |
| (1,1420) | 1:21:A:VAL:HG21 | 1:19:A:ILE:HD13 | 9        | 0.11          |
| (1,1420) | 1:21:A:VAL:HG22 | 1:19:A:ILE:HD11 | 9        | 0.11          |
| (1,1420) | 1:21:A:VAL:HG22 | 1:19:A:ILE:HD12 | 9        | 0.11          |
| (1,1420) | 1:21:A:VAL:HG22 | 1:19:A:ILE:HD13 | 9        | 0.11          |
| (1,1420) | 1:21:A:VAL:HG23 | 1:19:A:ILE:HD11 | 9        | 0.11          |
| (1,1420) | 1:21:A:VAL:HG23 | 1:19:A:ILE:HD12 | 9        | 0.11          |
| (1,1420) | 1:21:A:VAL:HG23 | 1:19:A:ILE:HD13 | 9        | 0.11          |
| (1,1420) | 1:21:A:VAL:HG21 | 1:19:A:ILE:HD11 | 15       | 0.11          |
| (1,1420) | 1:21:A:VAL:HG21 | 1:19:A:ILE:HD12 | 15       | 0.11          |
| (1,1420) | 1:21:A:VAL:HG21 | 1:19:A:ILE:HD13 | 15       | 0.11          |
| (1,1420) | 1:21:A:VAL:HG22 | 1:19:A:ILE:HD11 | 15       | 0.11          |
| (1,1420) | 1:21:A:VAL:HG22 | 1:19:A:ILE:HD12 | 15       | 0.11          |
| (1,1420) | 1:21:A:VAL:HG22 | 1:19:A:ILE:HD13 | 15       | 0.11          |
| (1,1420) | 1:21:A:VAL:HG23 | 1:19:A:ILE:HD11 | 15       | 0.11          |
| (1,1420) | 1:21:A:VAL:HG23 | 1:19:A:ILE:HD12 | 15       | 0.11          |
| (1,1420) | 1:21:A:VAL:HG23 | 1:19:A:ILE:HD13 | 15       | 0.11          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1418) | 1:21:A:VAL:HG11 | 1:27:A:ALA:HB1 | 9        | 0.11          |
| (1,1418) | 1:21:A:VAL:HG11 | 1:27:A:ALA:HB2 | 9        | 0.11          |
| (1,1418) | 1:21:A:VAL:HG11 | 1:27:A:ALA:HB3 | 9        | 0.11          |
| (1,1418) | 1:21:A:VAL:HG12 | 1:27:A:ALA:HB1 | 9        | 0.11          |
| (1,1418) | 1:21:A:VAL:HG12 | 1:27:A:ALA:HB2 | 9        | 0.11          |
| (1,1418) | 1:21:A:VAL:HG12 | 1:27:A:ALA:HB3 | 9        | 0.11          |
| (1,1418) | 1:21:A:VAL:HG13 | 1:27:A:ALA:HB1 | 9        | 0.11          |
| (1,1418) | 1:21:A:VAL:HG13 | 1:27:A:ALA:HB2 | 9        | 0.11          |
| (1,1418) | 1:21:A:VAL:HG13 | 1:27:A:ALA:HB3 | 9        | 0.11          |
| (1,1403) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H   | 7        | 0.11          |
| (1,1403) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H   | 7        | 0.11          |
| (1,1403) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H   | 7        | 0.11          |
| (1,1403) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H   | 9        | 0.11          |
| (1,1403) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H   | 9        | 0.11          |
| (1,1403) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H   | 9        | 0.11          |
| (1,1403) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H   | 21       | 0.11          |
| (1,1403) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H   | 21       | 0.11          |
| (1,1403) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H   | 21       | 0.11          |
| (1,1403) | 1:95:A:ALA:HB1  | 1:18:A:ASN:H   | 37       | 0.11          |
| (1,1403) | 1:95:A:ALA:HB2  | 1:18:A:ASN:H   | 37       | 0.11          |
| (1,1403) | 1:95:A:ALA:HB3  | 1:18:A:ASN:H   | 37       | 0.11          |
| (1,1401) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H   | 14       | 0.11          |
| (1,1401) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H   | 14       | 0.11          |
| (1,1401) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H   | 14       | 0.11          |
| (1,1401) | 1:95:A:ALA:HB1  | 1:96:A:GLU:H   | 27       | 0.11          |
| (1,1401) | 1:95:A:ALA:HB2  | 1:96:A:GLU:H   | 27       | 0.11          |
| (1,1401) | 1:95:A:ALA:HB3  | 1:96:A:GLU:H   | 27       | 0.11          |
| (1,1396) | 1:95:A:ALA:HB1  | 1:94:A:THR:HA  | 28       | 0.11          |
| (1,1396) | 1:95:A:ALA:HB2  | 1:94:A:THR:HA  | 28       | 0.11          |
| (1,1396) | 1:95:A:ALA:HB3  | 1:94:A:THR:HA  | 28       | 0.11          |
| (1,1387) | 1:91:A:ALA:HB1  | 1:12:A:PHE:HZ  | 16       | 0.11          |
| (1,1387) | 1:91:A:ALA:HB2  | 1:12:A:PHE:HZ  | 16       | 0.11          |
| (1,1387) | 1:91:A:ALA:HB3  | 1:12:A:PHE:HZ  | 16       | 0.11          |
| (1,1387) | 1:91:A:ALA:HB1  | 1:12:A:PHE:HZ  | 26       | 0.11          |
| (1,1387) | 1:91:A:ALA:HB2  | 1:12:A:PHE:HZ  | 26       | 0.11          |
| (1,1387) | 1:91:A:ALA:HB3  | 1:12:A:PHE:HZ  | 26       | 0.11          |
| (1,1384) | 1:91:A:ALA:HB1  | 1:83:A:ALA:HB1 | 5        | 0.11          |
| (1,1384) | 1:91:A:ALA:HB1  | 1:83:A:ALA:HB2 | 5        | 0.11          |
| (1,1384) | 1:91:A:ALA:HB1  | 1:83:A:ALA:HB3 | 5        | 0.11          |
| (1,1384) | 1:91:A:ALA:HB2  | 1:83:A:ALA:HB1 | 5        | 0.11          |
| (1,1384) | 1:91:A:ALA:HB2  | 1:83:A:ALA:HB2 | 5        | 0.11          |
| (1,1384) | 1:91:A:ALA:HB2  | 1:83:A:ALA:HB3 | 5        | 0.11          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 5        | 0.11          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 5        | 0.11          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 5        | 0.11          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 9        | 0.11          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 9        | 0.11          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 9        | 0.11          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 9        | 0.11          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 9        | 0.11          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 9        | 0.11          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 9        | 0.11          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 9        | 0.11          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 9        | 0.11          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 14       | 0.11          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 14       | 0.11          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 14       | 0.11          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 14       | 0.11          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 14       | 0.11          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 14       | 0.11          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 14       | 0.11          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 14       | 0.11          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 14       | 0.11          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 19       | 0.11          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 19       | 0.11          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 19       | 0.11          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 19       | 0.11          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 19       | 0.11          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 19       | 0.11          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 19       | 0.11          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 19       | 0.11          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 19       | 0.11          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB1 | 22       | 0.11          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB2 | 22       | 0.11          |
| (1,1384) | 1:91:A:ALA:HB1 | 1:83:A:ALA:HB3 | 22       | 0.11          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB1 | 22       | 0.11          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB2 | 22       | 0.11          |
| (1,1384) | 1:91:A:ALA:HB2 | 1:83:A:ALA:HB3 | 22       | 0.11          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB1 | 22       | 0.11          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB2 | 22       | 0.11          |
| (1,1384) | 1:91:A:ALA:HB3 | 1:83:A:ALA:HB3 | 22       | 0.11          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 5        | 0.11          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 5        | 0.11          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 5        | 0.11          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 5        | 0.11          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 5        | 0.11          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 5        | 0.11          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 5        | 0.11          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 5        | 0.11          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 5        | 0.11          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 9        | 0.11          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 9        | 0.11          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 9        | 0.11          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 9        | 0.11          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 9        | 0.11          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 9        | 0.11          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 9        | 0.11          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 9        | 0.11          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 9        | 0.11          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 14       | 0.11          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 14       | 0.11          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 14       | 0.11          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 14       | 0.11          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 14       | 0.11          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 14       | 0.11          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 14       | 0.11          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 14       | 0.11          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 14       | 0.11          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 19       | 0.11          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 19       | 0.11          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 19       | 0.11          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 19       | 0.11          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 19       | 0.11          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 19       | 0.11          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 19       | 0.11          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 19       | 0.11          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 19       | 0.11          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB1 | 22       | 0.11          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB2 | 22       | 0.11          |
| (1,1379) | 1:83:A:ALA:HB1 | 1:91:A:ALA:HB3 | 22       | 0.11          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB1 | 22       | 0.11          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB2 | 22       | 0.11          |
| (1,1379) | 1:83:A:ALA:HB2 | 1:91:A:ALA:HB3 | 22       | 0.11          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB1 | 22       | 0.11          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB2 | 22       | 0.11          |
| (1,1379) | 1:83:A:ALA:HB3 | 1:91:A:ALA:HB3 | 22       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1357) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 7        | 0.11          |
| (1,1357) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 7        | 0.11          |
| (1,1357) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 7        | 0.11          |
| (1,1357) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 10       | 0.11          |
| (1,1357) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 10       | 0.11          |
| (1,1357) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 10       | 0.11          |
| (1,1357) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 15       | 0.11          |
| (1,1357) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 15       | 0.11          |
| (1,1357) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 15       | 0.11          |
| (1,1357) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 16       | 0.11          |
| (1,1357) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 16       | 0.11          |
| (1,1357) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 16       | 0.11          |
| (1,1357) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 22       | 0.11          |
| (1,1357) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 22       | 0.11          |
| (1,1357) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 22       | 0.11          |
| (1,1357) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 27       | 0.11          |
| (1,1357) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 27       | 0.11          |
| (1,1357) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 27       | 0.11          |
| (1,1357) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 28       | 0.11          |
| (1,1357) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 28       | 0.11          |
| (1,1357) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 28       | 0.11          |
| (1,1357) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 29       | 0.11          |
| (1,1357) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 29       | 0.11          |
| (1,1357) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 29       | 0.11          |
| (1,1357) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 37       | 0.11          |
| (1,1357) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 37       | 0.11          |
| (1,1357) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 37       | 0.11          |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H    | 2        | 0.11          |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H    | 2        | 0.11          |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H    | 2        | 0.11          |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H    | 5        | 0.11          |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H    | 5        | 0.11          |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H    | 5        | 0.11          |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H    | 6        | 0.11          |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H    | 6        | 0.11          |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H    | 6        | 0.11          |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H    | 9        | 0.11          |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H    | 9        | 0.11          |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H    | 9        | 0.11          |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H    | 11       | 0.11          |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H    | 11       | 0.11          |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H    | 11       | 0.11          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H  | 22       | 0.11          |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H  | 22       | 0.11          |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H  | 22       | 0.11          |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H  | 23       | 0.11          |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H  | 23       | 0.11          |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H  | 23       | 0.11          |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H  | 25       | 0.11          |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H  | 25       | 0.11          |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H  | 25       | 0.11          |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H  | 32       | 0.11          |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H  | 32       | 0.11          |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H  | 32       | 0.11          |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H  | 39       | 0.11          |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H  | 39       | 0.11          |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H  | 39       | 0.11          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 3        | 0.11          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 3        | 0.11          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 3        | 0.11          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 6        | 0.11          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 6        | 0.11          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 6        | 0.11          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 14       | 0.11          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 14       | 0.11          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 14       | 0.11          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 15       | 0.11          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 15       | 0.11          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 15       | 0.11          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 19       | 0.11          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 19       | 0.11          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 19       | 0.11          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 20       | 0.11          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 20       | 0.11          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 20       | 0.11          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 23       | 0.11          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 23       | 0.11          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 23       | 0.11          |
| (1,1343) | 1:16:A:ILE:HD11 | 1:16:A:ILE:HA | 40       | 0.11          |
| (1,1343) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HA | 40       | 0.11          |
| (1,1343) | 1:16:A:ILE:HD13 | 1:16:A:ILE:HA | 40       | 0.11          |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H  | 7        | 0.11          |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H  | 8        | 0.11          |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H  | 14       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 21       | 0.11          |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 25       | 0.11          |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 30       | 0.11          |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 33       | 0.11          |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 37       | 0.11          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 22       | 0.11          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 22       | 0.11          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 22       | 0.11          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 32       | 0.11          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 32       | 0.11          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 32       | 0.11          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 33       | 0.11          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 33       | 0.11          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 33       | 0.11          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG21 | 37       | 0.11          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG22 | 37       | 0.11          |
| (1,1291) | 1:40:A:VAL:HB   | 1:81:A:VAL:HG23 | 37       | 0.11          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1  | 2        | 0.11          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2  | 2        | 0.11          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3  | 2        | 0.11          |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1  | 2        | 0.11          |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2  | 2        | 0.11          |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3  | 2        | 0.11          |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1  | 2        | 0.11          |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2  | 2        | 0.11          |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3  | 2        | 0.11          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1  | 13       | 0.11          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2  | 13       | 0.11          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3  | 13       | 0.11          |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1  | 13       | 0.11          |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2  | 13       | 0.11          |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3  | 13       | 0.11          |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1  | 13       | 0.11          |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2  | 13       | 0.11          |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3  | 13       | 0.11          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB1  | 14       | 0.11          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB2  | 14       | 0.11          |
| (1,1290) | 1:40:A:VAL:HG21 | 1:83:A:ALA:HB3  | 14       | 0.11          |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB1  | 14       | 0.11          |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB2  | 14       | 0.11          |
| (1,1290) | 1:40:A:VAL:HG22 | 1:83:A:ALA:HB3  | 14       | 0.11          |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB1  | 14       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB2  | 14       | 0.11          |
| (1,1290) | 1:40:A:VAL:HG23 | 1:83:A:ALA:HB3  | 14       | 0.11          |
| (1,1289) | 1:40:A:VAL:HG21 | 1:42:A:TRP:HE1  | 12       | 0.11          |
| (1,1289) | 1:40:A:VAL:HG22 | 1:42:A:TRP:HE1  | 12       | 0.11          |
| (1,1289) | 1:40:A:VAL:HG23 | 1:42:A:TRP:HE1  | 12       | 0.11          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 22       | 0.11          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 22       | 0.11          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 22       | 0.11          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 32       | 0.11          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 32       | 0.11          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 32       | 0.11          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 33       | 0.11          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 33       | 0.11          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 33       | 0.11          |
| (1,1278) | 1:81:A:VAL:HG21 | 1:40:A:VAL:HB   | 37       | 0.11          |
| (1,1278) | 1:81:A:VAL:HG22 | 1:40:A:VAL:HB   | 37       | 0.11          |
| (1,1278) | 1:81:A:VAL:HG23 | 1:40:A:VAL:HB   | 37       | 0.11          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG11 | 16       | 0.11          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG12 | 16       | 0.11          |
| (1,1268) | 1:94:A:THR:HG21 | 1:78:A:VAL:HG13 | 16       | 0.11          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG11 | 16       | 0.11          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG12 | 16       | 0.11          |
| (1,1268) | 1:94:A:THR:HG22 | 1:78:A:VAL:HG13 | 16       | 0.11          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG11 | 16       | 0.11          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG12 | 16       | 0.11          |
| (1,1268) | 1:94:A:THR:HG23 | 1:78:A:VAL:HG13 | 16       | 0.11          |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 31       | 0.11          |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 31       | 0.11          |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 31       | 0.11          |
| (1,1261) | 1:67:A:THR:HG21 | 1:56:A:ASN:H    | 11       | 0.11          |
| (1,1261) | 1:67:A:THR:HG22 | 1:56:A:ASN:H    | 11       | 0.11          |
| (1,1261) | 1:67:A:THR:HG23 | 1:56:A:ASN:H    | 11       | 0.11          |
| (1,1261) | 1:67:A:THR:HG21 | 1:56:A:ASN:H    | 22       | 0.11          |
| (1,1261) | 1:67:A:THR:HG22 | 1:56:A:ASN:H    | 22       | 0.11          |
| (1,1261) | 1:67:A:THR:HG23 | 1:56:A:ASN:H    | 22       | 0.11          |
| (1,1261) | 1:67:A:THR:HG21 | 1:56:A:ASN:H    | 25       | 0.11          |
| (1,1261) | 1:67:A:THR:HG22 | 1:56:A:ASN:H    | 25       | 0.11          |
| (1,1261) | 1:67:A:THR:HG23 | 1:56:A:ASN:H    | 25       | 0.11          |
| (1,1261) | 1:67:A:THR:HG21 | 1:56:A:ASN:H    | 30       | 0.11          |
| (1,1261) | 1:67:A:THR:HG22 | 1:56:A:ASN:H    | 30       | 0.11          |
| (1,1261) | 1:67:A:THR:HG23 | 1:56:A:ASN:H    | 30       | 0.11          |
| (1,1248) | 1:28:A:THR:HG21 | 1:67:A:THR:HG21 | 34       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1248) | 1:28:A:THR:HG21 | 1:67:A:THR:HG22 | 34       | 0.11          |
| (1,1248) | 1:28:A:THR:HG21 | 1:67:A:THR:HG23 | 34       | 0.11          |
| (1,1248) | 1:28:A:THR:HG22 | 1:67:A:THR:HG21 | 34       | 0.11          |
| (1,1248) | 1:28:A:THR:HG22 | 1:67:A:THR:HG22 | 34       | 0.11          |
| (1,1248) | 1:28:A:THR:HG22 | 1:67:A:THR:HG23 | 34       | 0.11          |
| (1,1248) | 1:28:A:THR:HG23 | 1:67:A:THR:HG21 | 34       | 0.11          |
| (1,1248) | 1:28:A:THR:HG23 | 1:67:A:THR:HG22 | 34       | 0.11          |
| (1,1248) | 1:28:A:THR:HG23 | 1:67:A:THR:HG23 | 34       | 0.11          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 4        | 0.11          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 4        | 0.11          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 4        | 0.11          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 11       | 0.11          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 11       | 0.11          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 11       | 0.11          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 16       | 0.11          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 16       | 0.11          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 16       | 0.11          |
| (1,1244) | 1:28:A:THR:HG21 | 1:30:A:GLU:H    | 27       | 0.11          |
| (1,1244) | 1:28:A:THR:HG22 | 1:30:A:GLU:H    | 27       | 0.11          |
| (1,1244) | 1:28:A:THR:HG23 | 1:30:A:GLU:H    | 27       | 0.11          |
| (1,1239) | 1:13:A:THR:HG21 | 1:34:A:SER:H    | 7        | 0.11          |
| (1,1239) | 1:13:A:THR:HG22 | 1:34:A:SER:H    | 7        | 0.11          |
| (1,1239) | 1:13:A:THR:HG23 | 1:34:A:SER:H    | 7        | 0.11          |
| (1,1239) | 1:13:A:THR:HG21 | 1:34:A:SER:H    | 40       | 0.11          |
| (1,1239) | 1:13:A:THR:HG22 | 1:34:A:SER:H    | 40       | 0.11          |
| (1,1239) | 1:13:A:THR:HG23 | 1:34:A:SER:H    | 40       | 0.11          |
| (1,1236) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3  | 2        | 0.11          |
| (1,1236) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3  | 2        | 0.11          |
| (1,1236) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3  | 2        | 0.11          |
| (1,1236) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3  | 12       | 0.11          |
| (1,1236) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3  | 12       | 0.11          |
| (1,1236) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3  | 12       | 0.11          |
| (1,1236) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3  | 19       | 0.11          |
| (1,1236) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3  | 19       | 0.11          |
| (1,1236) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3  | 19       | 0.11          |
| (1,1226) | 1:101:A:LEU:H   | 1:22:A:SER:HA   | 3        | 0.11          |
| (1,1226) | 1:101:A:LEU:H   | 1:22:A:SER:HA   | 13       | 0.11          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 2        | 0.11          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 2        | 0.11          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 2        | 0.11          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 5        | 0.11          |
| (1,1222) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 5        | 0.11          |

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| Key      | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|----------|--------------|-----------------|----------|---------------|
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD23 | 5        | 0.11          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD21 | 21       | 0.11          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD22 | 21       | 0.11          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD23 | 21       | 0.11          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD21 | 24       | 0.11          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD22 | 24       | 0.11          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD23 | 24       | 0.11          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD21 | 30       | 0.11          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD22 | 30       | 0.11          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD23 | 30       | 0.11          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD21 | 31       | 0.11          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD22 | 31       | 0.11          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD23 | 31       | 0.11          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD21 | 32       | 0.11          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD22 | 32       | 0.11          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD23 | 32       | 0.11          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD21 | 33       | 0.11          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD22 | 33       | 0.11          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD23 | 33       | 0.11          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD21 | 35       | 0.11          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD22 | 35       | 0.11          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD23 | 35       | 0.11          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD21 | 36       | 0.11          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD22 | 36       | 0.11          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD23 | 36       | 0.11          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD21 | 38       | 0.11          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD22 | 38       | 0.11          |
| (1,1222) | 1:97:A:LEU:H | 1:97:A:LEU:HD23 | 38       | 0.11          |
| (1,1217) | 1:69:A:HIS:H | 1:56:A:ASN:H    | 31       | 0.11          |
| (1,1217) | 1:69:A:HIS:H | 1:56:A:ASN:H    | 34       | 0.11          |
| (1,1217) | 1:69:A:HIS:H | 1:56:A:ASN:H    | 40       | 0.11          |
| (1,1213) | 1:66:A:MET:H | 1:28:A:THR:HA   | 8        | 0.11          |
| (1,1213) | 1:66:A:MET:H | 1:28:A:THR:HA   | 9        | 0.11          |
| (1,1213) | 1:66:A:MET:H | 1:28:A:THR:HA   | 30       | 0.11          |
| (1,1213) | 1:66:A:MET:H | 1:28:A:THR:HA   | 33       | 0.11          |
| (1,1213) | 1:66:A:MET:H | 1:28:A:THR:HA   | 34       | 0.11          |
| (1,1213) | 1:66:A:MET:H | 1:28:A:THR:HA   | 40       | 0.11          |
| (1,1208) | 1:56:A:ASN:H | 1:66:A:MET:HG2  | 32       | 0.11          |
| (1,1204) | 1:42:A:TRP:H | 1:57:A:PHE:HE1  | 7        | 0.11          |
| (1,1204) | 1:42:A:TRP:H | 1:57:A:PHE:HE2  | 7        | 0.11          |
| (1,1204) | 1:42:A:TRP:H | 1:57:A:PHE:HE1  | 29       | 0.11          |
| (1,1204) | 1:42:A:TRP:H | 1:57:A:PHE:HE2  | 29       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1204) | 1:42:A:TRP:H    | 1:57:A:PHE:HE1  | 39       | 0.11          |
| (1,1204) | 1:42:A:TRP:H    | 1:57:A:PHE:HE2  | 39       | 0.11          |
| (1,1197) | 1:33:A:VAL:H    | 1:63:A:CYS:HA   | 4        | 0.11          |
| (1,1176) | 1:47:A:THR:H    | 1:44:A:LYS:HB3  | 3        | 0.11          |
| (1,1176) | 1:47:A:THR:H    | 1:44:A:LYS:HB3  | 22       | 0.11          |
| (1,1176) | 1:47:A:THR:H    | 1:44:A:LYS:HB3  | 24       | 0.11          |
| (1,1176) | 1:47:A:THR:H    | 1:44:A:LYS:HB3  | 40       | 0.11          |
| (1,1149) | 1:54:A:LYS:H    | 1:53:A:GLN:HG3  | 4        | 0.11          |
| (1,1149) | 1:54:A:LYS:H    | 1:53:A:GLN:HG3  | 13       | 0.11          |
| (1,1149) | 1:54:A:LYS:H    | 1:53:A:GLN:HG3  | 39       | 0.11          |
| (1,1149) | 1:54:A:LYS:H    | 1:53:A:GLN:HG3  | 40       | 0.11          |
| (1,1130) | 1:40:A:VAL:H    | 1:83:A:ALA:HB1  | 7        | 0.11          |
| (1,1130) | 1:40:A:VAL:H    | 1:83:A:ALA:HB2  | 7        | 0.11          |
| (1,1130) | 1:40:A:VAL:H    | 1:83:A:ALA:HB3  | 7        | 0.11          |
| (1,1064) | 1:71:A:VAL:H    | 1:25:A:GLN:H    | 5        | 0.11          |
| (1,1052) | 1:26:A:SER:H    | 1:25:A:GLN:HG2  | 17       | 0.11          |
| (1,1037) | 1:56:A:ASN:HD22 | 1:56:A:ASN:HA   | 7        | 0.11          |
| (1,1020) | 1:48:A:GLU:H    | 1:48:A:GLU:HG3  | 1        | 0.11          |
| (1,1020) | 1:48:A:GLU:H    | 1:48:A:GLU:HG3  | 4        | 0.11          |
| (1,1020) | 1:48:A:GLU:H    | 1:48:A:GLU:HG3  | 23       | 0.11          |
| (1,1020) | 1:48:A:GLU:H    | 1:48:A:GLU:HG3  | 26       | 0.11          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG21 | 3        | 0.11          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG22 | 3        | 0.11          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG23 | 3        | 0.11          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG21 | 4        | 0.11          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG22 | 4        | 0.11          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG23 | 4        | 0.11          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG21 | 15       | 0.11          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG22 | 15       | 0.11          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG23 | 15       | 0.11          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG21 | 22       | 0.11          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG22 | 22       | 0.11          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG23 | 22       | 0.11          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG21 | 25       | 0.11          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG22 | 25       | 0.11          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG23 | 25       | 0.11          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG21 | 30       | 0.11          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG22 | 30       | 0.11          |
| (1,997)  | 1:79:A:TYR:H    | 1:94:A:THR:HG23 | 30       | 0.11          |
| (1,987)  | 1:12:A:PHE:H    | 1:11:A:GLN:HB2  | 3        | 0.11          |
| (1,987)  | 1:12:A:PHE:H    | 1:11:A:GLN:HB2  | 4        | 0.11          |
| (1,987)  | 1:12:A:PHE:H    | 1:11:A:GLN:HB2  | 8        | 0.11          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,987) | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 14       | 0.11          |
| (1,987) | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 15       | 0.11          |
| (1,987) | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 17       | 0.11          |
| (1,967) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 14       | 0.11          |
| (1,967) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 16       | 0.11          |
| (1,967) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 27       | 0.11          |
| (1,967) | 1:21:A:VAL:H | 1:99:A:GLY:HA3  | 28       | 0.11          |
| (1,941) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 12       | 0.11          |
| (1,941) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 17       | 0.11          |
| (1,941) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 18       | 0.11          |
| (1,941) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 24       | 0.11          |
| (1,941) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 26       | 0.11          |
| (1,941) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 36       | 0.11          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 3        | 0.11          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 3        | 0.11          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 3        | 0.11          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 6        | 0.11          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 6        | 0.11          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 6        | 0.11          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 8        | 0.11          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 8        | 0.11          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 8        | 0.11          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 16       | 0.11          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 16       | 0.11          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 16       | 0.11          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 25       | 0.11          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 25       | 0.11          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 25       | 0.11          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 29       | 0.11          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 29       | 0.11          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 29       | 0.11          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 32       | 0.11          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 32       | 0.11          |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 32       | 0.11          |
| (1,899) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 3        | 0.11          |
| (1,899) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 10       | 0.11          |
| (1,899) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 13       | 0.11          |
| (1,899) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 15       | 0.11          |
| (1,899) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 18       | 0.11          |
| (1,899) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 26       | 0.11          |
| (1,899) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 27       | 0.11          |
| (1,899) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 29       | 0.11          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,899) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 32       | 0.11          |
| (1,899) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 35       | 0.11          |
| (1,899) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 37       | 0.11          |
| (1,889) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 2        | 0.11          |
| (1,889) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 5        | 0.11          |
| (1,889) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 11       | 0.11          |
| (1,889) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 12       | 0.11          |
| (1,889) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 17       | 0.11          |
| (1,889) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 19       | 0.11          |
| (1,889) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 25       | 0.11          |
| (1,889) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 26       | 0.11          |
| (1,889) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 36       | 0.11          |
| (1,888) | 1:80:A:SER:H | 1:43:A:TYR:HB3  | 38       | 0.11          |
| (1,879) | 1:30:A:GLU:H | 1:29:A:PHE:HB2  | 12       | 0.11          |
| (1,863) | 1:86:A:GLU:H | 1:85:A:LEU:HB3  | 29       | 0.11          |
| (1,863) | 1:86:A:GLU:H | 1:85:A:LEU:HB3  | 34       | 0.11          |
| (1,860) | 1:86:A:GLU:H | 1:85:A:LEU:HA   | 3        | 0.11          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 11       | 0.11          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 11       | 0.11          |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 11       | 0.11          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG21 | 17       | 0.11          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG22 | 17       | 0.11          |
| (1,814) | 1:25:A:GLN:H | 1:71:A:VAL:HG23 | 17       | 0.11          |
| (1,813) | 1:25:A:GLN:H | 1:25:A:GLN:HG3  | 4        | 0.11          |
| (1,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB   | 13       | 0.11          |
| (1,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB   | 19       | 0.11          |
| (1,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB   | 25       | 0.11          |
| (1,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB   | 27       | 0.11          |
| (1,742) | 1:76:A:GLU:H | 1:77:A:GLY:H    | 3        | 0.11          |
| (1,742) | 1:76:A:GLU:H | 1:77:A:GLY:H    | 10       | 0.11          |
| (1,742) | 1:76:A:GLU:H | 1:77:A:GLY:H    | 14       | 0.11          |
| (1,742) | 1:76:A:GLU:H | 1:77:A:GLY:H    | 16       | 0.11          |
| (1,742) | 1:76:A:GLU:H | 1:77:A:GLY:H    | 17       | 0.11          |
| (1,726) | 1:49:A:LEU:H | 1:48:A:GLU:HG3  | 4        | 0.11          |
| (1,726) | 1:49:A:LEU:H | 1:48:A:GLU:HG3  | 5        | 0.11          |
| (1,726) | 1:49:A:LEU:H | 1:48:A:GLU:HG3  | 19       | 0.11          |
| (1,726) | 1:49:A:LEU:H | 1:48:A:GLU:HG3  | 21       | 0.11          |
| (1,726) | 1:49:A:LEU:H | 1:48:A:GLU:HG3  | 32       | 0.11          |
| (1,726) | 1:49:A:LEU:H | 1:48:A:GLU:HG3  | 34       | 0.11          |
| (1,726) | 1:49:A:LEU:H | 1:48:A:GLU:HG3  | 36       | 0.11          |
| (1,709) | 1:16:A:ILE:H | 1:31:A:CYS:HB2  | 11       | 0.11          |
| (1,709) | 1:16:A:ILE:H | 1:31:A:CYS:HB2  | 14       | 0.11          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,709) | 1:16:A:ILE:H  | 1:31:A:CYS:HB2  | 25       | 0.11          |
| (1,709) | 1:16:A:ILE:H  | 1:31:A:CYS:HB2  | 35       | 0.11          |
| (1,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 2        | 0.11          |
| (1,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 3        | 0.11          |
| (1,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 4        | 0.11          |
| (1,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 5        | 0.11          |
| (1,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 6        | 0.11          |
| (1,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 11       | 0.11          |
| (1,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 12       | 0.11          |
| (1,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 13       | 0.11          |
| (1,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 14       | 0.11          |
| (1,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 15       | 0.11          |
| (1,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 16       | 0.11          |
| (1,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 21       | 0.11          |
| (1,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 22       | 0.11          |
| (1,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 25       | 0.11          |
| (1,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 26       | 0.11          |
| (1,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 32       | 0.11          |
| (1,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 37       | 0.11          |
| (1,666) | 1:72:A:THR:H  | 1:72:A:THR:HB   | 38       | 0.11          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 1        | 0.11          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 3        | 0.11          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 8        | 0.11          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 21       | 0.11          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 25       | 0.11          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 28       | 0.11          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 31       | 0.11          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 32       | 0.11          |
| (1,653) | 1:100:A:GLU:H | 1:100:A:GLU:HG2 | 38       | 0.11          |
| (1,650) | 1:100:A:GLU:H | 1:99:A:GLY:HA3  | 22       | 0.11          |
| (1,609) | 1:43:A:TYR:H  | 1:42:A:TRP:HB2  | 10       | 0.11          |
| (1,595) | 1:3:A:ASP:H   | 1:2:A:ILE:HG21  | 14       | 0.11          |
| (1,595) | 1:3:A:ASP:H   | 1:2:A:ILE:HG22  | 14       | 0.11          |
| (1,595) | 1:3:A:ASP:H   | 1:2:A:ILE:HG23  | 14       | 0.11          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 9        | 0.11          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 9        | 0.11          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 9        | 0.11          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 17       | 0.11          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 17       | 0.11          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG23 | 17       | 0.11          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG21 | 28       | 0.11          |
| (1,567) | 1:47:A:THR:H  | 1:47:A:THR:HG22 | 28       | 0.11          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 28       | 0.11          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 29       | 0.11          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 29       | 0.11          |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 29       | 0.11          |
| (1,558) | 1:47:A:THR:H | 1:43:A:TYR:HD1  | 18       | 0.11          |
| (1,558) | 1:47:A:THR:H | 1:43:A:TYR:HD2  | 18       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 2        | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 2        | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 2        | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 4        | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 4        | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 4        | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 5        | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 5        | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 5        | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 7        | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 7        | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 7        | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 8        | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 8        | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 8        | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 10       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 10       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 10       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 13       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 13       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 13       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 14       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 14       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 14       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 15       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 15       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 15       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 17       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 17       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 17       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 21       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 21       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 21       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 22       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 22       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 22       | 0.11          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 24       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 24       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 24       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 25       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 25       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 25       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 26       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 26       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 26       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 28       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 28       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 28       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 30       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 30       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 30       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 31       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 31       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 31       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 32       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 32       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 32       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 34       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 34       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 34       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 36       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 36       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 36       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 37       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 37       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 37       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 38       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 38       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 38       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 39       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 39       | 0.11          |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 39       | 0.11          |
| (1,549) | 1:71:A:VAL:H | 1:70:A:ASN:HB2  | 26       | 0.11          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 2        | 0.11          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 3        | 0.11          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 6        | 0.11          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 9        | 0.11          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 10       | 0.11          |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 11       | 0.11          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 15       | 0.11          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 19       | 0.11          |
| (1,547) | 1:71:A:VAL:H | 1:71:A:VAL:HA   | 28       | 0.11          |
| (1,546) | 1:71:A:VAL:H | 1:24:A:HIS:HA   | 9        | 0.11          |
| (1,531) | 1:99:A:GLY:H | 1:98:A:LYS:HG2  | 9        | 0.11          |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 5        | 0.11          |
| (1,528) | 1:99:A:GLY:H | 1:98:A:LYS:HB2  | 7        | 0.11          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 2        | 0.11          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 7        | 0.11          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 12       | 0.11          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 16       | 0.11          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 24       | 0.11          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 33       | 0.11          |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 40       | 0.11          |
| (1,419) | 1:69:A:HIS:H | 1:54:A:LYS:HA   | 40       | 0.11          |
| (1,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD21 | 22       | 0.11          |
| (1,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD22 | 22       | 0.11          |
| (1,404) | 1:77:A:GLY:H | 1:97:A:LEU:HD23 | 22       | 0.11          |
| (1,393) | 1:77:A:GLY:H | 1:96:A:GLU:HA   | 14       | 0.11          |
| (1,393) | 1:77:A:GLY:H | 1:96:A:GLU:HA   | 28       | 0.11          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 7        | 0.11          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 7        | 0.11          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 7        | 0.11          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 9        | 0.11          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 9        | 0.11          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 9        | 0.11          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 21       | 0.11          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 21       | 0.11          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 21       | 0.11          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB1  | 37       | 0.11          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB2  | 37       | 0.11          |
| (1,370) | 1:18:A:ASN:H | 1:95:A:ALA:HB3  | 37       | 0.11          |
| (1,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 13       | 0.11          |
| (1,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 14       | 0.11          |
| (1,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 16       | 0.11          |
| (1,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 20       | 0.11          |
| (1,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 21       | 0.11          |
| (1,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 30       | 0.11          |
| (1,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 33       | 0.11          |
| (1,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD1  | 8        | 0.11          |
| (1,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD2  | 8        | 0.11          |

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| Key     | Atom-1       | Atom-2         | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (1,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD1 | 20       | 0.11          |
| (1,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD2 | 20       | 0.11          |
| (1,314) | 1:63:A:CYS:H | 1:64:A:HIS:HD2 | 8        | 0.11          |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3 | 12       | 0.11          |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3 | 29       | 0.11          |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3 | 38       | 0.11          |
| (1,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3 | 2        | 0.11          |
| (1,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3 | 4        | 0.11          |
| (1,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3 | 9        | 0.11          |
| (1,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3 | 16       | 0.11          |
| (1,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3 | 27       | 0.11          |
| (1,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3 | 31       | 0.11          |
| (1,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3 | 37       | 0.11          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 3        | 0.11          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 4        | 0.11          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 5        | 0.11          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 8        | 0.11          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 14       | 0.11          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 17       | 0.11          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 18       | 0.11          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 26       | 0.11          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 29       | 0.11          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 30       | 0.11          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 31       | 0.11          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 32       | 0.11          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 34       | 0.11          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 35       | 0.11          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 37       | 0.11          |
| (1,239) | 1:13:A:THR:H | 1:14:A:LYS:HA  | 40       | 0.11          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1 | 3        | 0.11          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2 | 3        | 0.11          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1 | 14       | 0.11          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2 | 14       | 0.11          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1 | 15       | 0.11          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2 | 15       | 0.11          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1 | 19       | 0.11          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2 | 19       | 0.11          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1 | 22       | 0.11          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2 | 22       | 0.11          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1 | 28       | 0.11          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2 | 28       | 0.11          |
| (1,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1 | 32       | 0.11          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD2  | 32       | 0.11          |
| (1,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD1  | 33       | 0.11          |
| (1,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD2  | 33       | 0.11          |
| (1,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD1  | 35       | 0.11          |
| (1,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD2  | 35       | 0.11          |
| (1,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD1  | 40       | 0.11          |
| (1,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD2  | 40       | 0.11          |
| (1,203) | 1:90:A:GLU:H  | 1:91:A:ALA:H    | 1        | 0.11          |
| (1,203) | 1:90:A:GLU:H  | 1:91:A:ALA:H    | 4        | 0.11          |
| (1,203) | 1:90:A:GLU:H  | 1:91:A:ALA:H    | 5        | 0.11          |
| (1,203) | 1:90:A:GLU:H  | 1:91:A:ALA:H    | 8        | 0.11          |
| (1,203) | 1:90:A:GLU:H  | 1:91:A:ALA:H    | 9        | 0.11          |
| (1,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 11       | 0.11          |
| (1,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 18       | 0.11          |
| (1,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 34       | 0.11          |
| (1,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 38       | 0.11          |
| (1,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 39       | 0.11          |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG21 | 9        | 0.11          |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG22 | 9        | 0.11          |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG23 | 9        | 0.11          |
| (1,198) | 1:90:A:GLU:H  | 1:90:A:GLU:HB2  | 15       | 0.11          |
| (1,182) | 1:11:A:GLN:H  | 1:10:A:ILE:HD11 | 1        | 0.11          |
| (1,182) | 1:11:A:GLN:H  | 1:10:A:ILE:HD12 | 1        | 0.11          |
| (1,182) | 1:11:A:GLN:H  | 1:10:A:ILE:HD13 | 1        | 0.11          |
| (1,182) | 1:11:A:GLN:H  | 1:10:A:ILE:HD11 | 3        | 0.11          |
| (1,182) | 1:11:A:GLN:H  | 1:10:A:ILE:HD12 | 3        | 0.11          |
| (1,182) | 1:11:A:GLN:H  | 1:10:A:ILE:HD13 | 3        | 0.11          |
| (1,182) | 1:11:A:GLN:H  | 1:10:A:ILE:HD11 | 8        | 0.11          |
| (1,182) | 1:11:A:GLN:H  | 1:10:A:ILE:HD12 | 8        | 0.11          |
| (1,182) | 1:11:A:GLN:H  | 1:10:A:ILE:HD13 | 8        | 0.11          |
| (1,182) | 1:11:A:GLN:H  | 1:10:A:ILE:HD11 | 20       | 0.11          |
| (1,182) | 1:11:A:GLN:H  | 1:10:A:ILE:HD12 | 20       | 0.11          |
| (1,182) | 1:11:A:GLN:H  | 1:10:A:ILE:HD13 | 20       | 0.11          |
| (1,165) | 1:10:A:ILE:H  | 1:9:A:PRO:HB2   | 8        | 0.11          |
| (1,165) | 1:10:A:ILE:H  | 1:9:A:PRO:HB2   | 9        | 0.11          |
| (1,165) | 1:10:A:ILE:H  | 1:9:A:PRO:HB2   | 11       | 0.11          |
| (1,165) | 1:10:A:ILE:H  | 1:9:A:PRO:HB2   | 13       | 0.11          |
| (1,165) | 1:10:A:ILE:H  | 1:9:A:PRO:HB2   | 17       | 0.11          |
| (1,148) | 1:45:A:GLY:H  | 1:46:A:PRO:HD2  | 27       | 0.11          |
| (1,142) | 1:101:A:LEU:H | 1:100:A:GLU:HB2 | 39       | 0.11          |
| (1,111) | 1:63:A:CYS:H  | 1:60:A:ASP:H    | 9        | 0.11          |
| (1,111) | 1:63:A:CYS:H  | 1:60:A:ASP:H    | 31       | 0.11          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,55)   | 1:42:A:TRP:H   | 1:42:A:TRP:HB3  | 1        | 0.11          |
| (1,55)   | 1:42:A:TRP:H   | 1:42:A:TRP:HB3  | 5        | 0.11          |
| (1,55)   | 1:42:A:TRP:H   | 1:42:A:TRP:HB3  | 18       | 0.11          |
| (1,55)   | 1:42:A:TRP:H   | 1:42:A:TRP:HB3  | 22       | 0.11          |
| (1,55)   | 1:42:A:TRP:H   | 1:42:A:TRP:HB3  | 34       | 0.11          |
| (1,49)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2  | 4        | 0.11          |
| (1,49)   | 1:57:A:PHE:H   | 1:56:A:ASN:HB2  | 19       | 0.11          |
| (1,37)   | 1:88:A:ARG:H   | 1:88:A:ARG:HB3  | 29       | 0.11          |
| (1,35)   | 1:88:A:ARG:H   | 1:88:A:ARG:HG2  | 25       | 0.11          |
| (1,35)   | 1:88:A:ARG:H   | 1:88:A:ARG:HG2  | 27       | 0.11          |
| (1,24)   | 1:89:A:GLY:H   | 1:9:A:PRO:HB3   | 16       | 0.11          |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 1        | 0.1           |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 1        | 0.1           |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 3        | 0.1           |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 3        | 0.1           |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 22       | 0.1           |
| (3,3215) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 22       | 0.1           |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG21 | 1        | 0.1           |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG22 | 1        | 0.1           |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG23 | 1        | 0.1           |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG21 | 32       | 0.1           |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG22 | 32       | 0.1           |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG23 | 32       | 0.1           |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG21 | 34       | 0.1           |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG22 | 34       | 0.1           |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG23 | 34       | 0.1           |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG21 | 35       | 0.1           |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG22 | 35       | 0.1           |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG23 | 35       | 0.1           |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG21 | 36       | 0.1           |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG22 | 36       | 0.1           |
| (3,3200) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG23 | 36       | 0.1           |
| (3,3191) | 1:43:A:TYR:HD1 | 1:44:A:LYS:H    | 2        | 0.1           |
| (3,3191) | 1:43:A:TYR:HD2 | 1:44:A:LYS:H    | 2        | 0.1           |
| (3,3191) | 1:43:A:TYR:HD1 | 1:44:A:LYS:H    | 6        | 0.1           |
| (3,3191) | 1:43:A:TYR:HD2 | 1:44:A:LYS:H    | 6        | 0.1           |
| (3,3189) | 1:43:A:TYR:HE1 | 1:82:A:ILE:HG13 | 14       | 0.1           |
| (3,3189) | 1:43:A:TYR:HE2 | 1:82:A:ILE:HG13 | 14       | 0.1           |
| (3,3189) | 1:43:A:TYR:HE1 | 1:82:A:ILE:HG13 | 17       | 0.1           |
| (3,3189) | 1:43:A:TYR:HE2 | 1:82:A:ILE:HG13 | 17       | 0.1           |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 3        | 0.1           |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 3        | 0.1           |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 3        | 0.1           |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 37       | 0.1           |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 37       | 0.1           |
| (3,3182) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 37       | 0.1           |
| (3,3164) | 1:42:A:TRP:HD1 | 1:41:A:THR:HA   | 10       | 0.1           |
| (3,3143) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3  | 5        | 0.1           |
| (3,3143) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 5        | 0.1           |
| (3,3143) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3  | 13       | 0.1           |
| (3,3143) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 13       | 0.1           |
| (3,3143) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3  | 21       | 0.1           |
| (3,3143) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 21       | 0.1           |
| (3,3143) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3  | 31       | 0.1           |
| (3,3143) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 31       | 0.1           |
| (3,3140) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2  | 40       | 0.1           |
| (3,3140) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2  | 40       | 0.1           |
| (3,3139) | 1:65:A:TYR:HE1 | 1:60:A:ASP:HB3  | 6        | 0.1           |
| (3,3139) | 1:65:A:TYR:HE2 | 1:60:A:ASP:HB3  | 6        | 0.1           |
| (3,3139) | 1:65:A:TYR:HE1 | 1:60:A:ASP:HB3  | 12       | 0.1           |
| (3,3139) | 1:65:A:TYR:HE2 | 1:60:A:ASP:HB3  | 12       | 0.1           |
| (3,3137) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3  | 18       | 0.1           |
| (3,3137) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3  | 18       | 0.1           |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 5        | 0.1           |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 5        | 0.1           |
| (3,3124) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 5        | 0.1           |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 5        | 0.1           |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 5        | 0.1           |
| (3,3124) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 5        | 0.1           |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 12       | 0.1           |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 12       | 0.1           |
| (3,3122) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 12       | 0.1           |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 12       | 0.1           |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 12       | 0.1           |
| (3,3122) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 12       | 0.1           |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 4        | 0.1           |
| (3,3106) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 4        | 0.1           |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 4        | 0.1           |
| (3,3106) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 4        | 0.1           |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE1  | 37       | 0.1           |
| (3,3098) | 1:66:A:MET:HE1 | 1:55:A:TYR:HE2  | 37       | 0.1           |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE1  | 37       | 0.1           |
| (3,3098) | 1:66:A:MET:HE2 | 1:55:A:TYR:HE2  | 37       | 0.1           |
| (3,3098) | 1:66:A:MET:HE3 | 1:55:A:TYR:HE1  | 37       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,3098) | 1:66:A:MET:HE3  | 1:55:A:TYR:HE2  | 37       | 0.1           |
| (3,3090) | 1:98:A:LYS:HD3  | 1:20:A:VAL:HG21 | 11       | 0.1           |
| (3,3090) | 1:98:A:LYS:HD3  | 1:20:A:VAL:HG22 | 11       | 0.1           |
| (3,3090) | 1:98:A:LYS:HD3  | 1:20:A:VAL:HG23 | 11       | 0.1           |
| (3,3088) | 1:97:A:LEU:HB3  | 1:29:A:PHE:HE1  | 4        | 0.1           |
| (3,3088) | 1:97:A:LEU:HB3  | 1:29:A:PHE:HE2  | 4        | 0.1           |
| (3,3088) | 1:97:A:LEU:HB3  | 1:29:A:PHE:HE1  | 20       | 0.1           |
| (3,3088) | 1:97:A:LEU:HB3  | 1:29:A:PHE:HE2  | 20       | 0.1           |
| (3,3088) | 1:97:A:LEU:HB3  | 1:29:A:PHE:HE1  | 27       | 0.1           |
| (3,3088) | 1:97:A:LEU:HB3  | 1:29:A:PHE:HE2  | 27       | 0.1           |
| (3,3048) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG21 | 12       | 0.1           |
| (3,3048) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG22 | 12       | 0.1           |
| (3,3048) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG23 | 12       | 0.1           |
| (3,3048) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG21 | 21       | 0.1           |
| (3,3048) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG22 | 21       | 0.1           |
| (3,3048) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG23 | 21       | 0.1           |
| (3,3048) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG21 | 40       | 0.1           |
| (3,3048) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG22 | 40       | 0.1           |
| (3,3048) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG23 | 40       | 0.1           |
| (3,3041) | 1:44:A:LYS:HE2  | 1:79:A:TYR:HE1  | 32       | 0.1           |
| (3,3041) | 1:44:A:LYS:HE2  | 1:79:A:TYR:HE2  | 32       | 0.1           |
| (3,3021) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 7        | 0.1           |
| (3,3021) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 7        | 0.1           |
| (3,3021) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 20       | 0.1           |
| (3,3021) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 20       | 0.1           |
| (3,3021) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 30       | 0.1           |
| (3,3021) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 30       | 0.1           |
| (3,3020) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG21 | 3        | 0.1           |
| (3,3020) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG22 | 3        | 0.1           |
| (3,3020) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG23 | 3        | 0.1           |
| (3,3020) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG21 | 14       | 0.1           |
| (3,3020) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG22 | 14       | 0.1           |
| (3,3020) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG23 | 14       | 0.1           |
| (3,3019) | 1:30:A:GLU:HB2  | 1:14:A:LYS:HE2  | 8        | 0.1           |
| (3,3019) | 1:30:A:GLU:HB2  | 1:14:A:LYS:HE2  | 12       | 0.1           |
| (3,3017) | 1:102:A:ARG:HD3 | 1:102:A:ARG:HB2 | 19       | 0.1           |
| (3,3004) | 1:15:A:ARG:HG2  | 1:93:A:SER:HB3  | 2        | 0.1           |
| (3,2982) | 1:65:A:TYR:HA   | 1:42:A:TRP:HZ2  | 2        | 0.1           |
| (3,2982) | 1:65:A:TYR:HA   | 1:42:A:TRP:HZ2  | 5        | 0.1           |
| (3,2982) | 1:65:A:TYR:HA   | 1:42:A:TRP:HZ2  | 27       | 0.1           |
| (3,2982) | 1:65:A:TYR:HA   | 1:42:A:TRP:HZ2  | 36       | 0.1           |
| (3,2981) | 1:88:A:ARG:HD2  | 1:35:A:PHE:HD1  | 19       | 0.1           |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,2981) | 1:88:A:ARG:HD2 | 1:35:A:PHE:HD2  | 19       | 0.1           |
| (3,2981) | 1:88:A:ARG:HD2 | 1:35:A:PHE:HD1  | 20       | 0.1           |
| (3,2981) | 1:88:A:ARG:HD2 | 1:35:A:PHE:HD2  | 20       | 0.1           |
| (3,2957) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA    | 31       | 0.1           |
| (3,2956) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HB2   | 16       | 0.1           |
| (3,2949) | 1:90:A:GLU:HA  | 1:84:A:ARG:HA   | 14       | 0.1           |
| (3,2947) | 1:44:A:LYS:HB2 | 1:47:A:THR:HG21 | 10       | 0.1           |
| (3,2947) | 1:44:A:LYS:HB2 | 1:47:A:THR:HG22 | 10       | 0.1           |
| (3,2947) | 1:44:A:LYS:HB2 | 1:47:A:THR:HG23 | 10       | 0.1           |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1  | 5        | 0.1           |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2  | 5        | 0.1           |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1  | 13       | 0.1           |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2  | 13       | 0.1           |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1  | 21       | 0.1           |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2  | 21       | 0.1           |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1  | 31       | 0.1           |
| (3,2944) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2  | 31       | 0.1           |
| (3,2938) | 1:26:A:SER:HA  | 1:70:A:ASN:H    | 7        | 0.1           |
| (3,2938) | 1:26:A:SER:HA  | 1:70:A:ASN:H    | 32       | 0.1           |
| (3,2937) | 1:17:A:GLN:HG2 | 1:18:A:ASN:H    | 7        | 0.1           |
| (3,2937) | 1:17:A:GLN:HG2 | 1:18:A:ASN:H    | 22       | 0.1           |
| (3,2917) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HG3  | 16       | 0.1           |
| (3,2917) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HG3  | 37       | 0.1           |
| (3,2848) | 1:84:A:ARG:HG2 | 1:84:A:ARG:HA   | 10       | 0.1           |
| (3,2848) | 1:84:A:ARG:HG2 | 1:84:A:ARG:HA   | 16       | 0.1           |
| (3,2848) | 1:84:A:ARG:HG2 | 1:84:A:ARG:HA   | 21       | 0.1           |
| (3,2848) | 1:84:A:ARG:HG2 | 1:84:A:ARG:HA   | 27       | 0.1           |
| (3,2848) | 1:84:A:ARG:HG2 | 1:84:A:ARG:HA   | 30       | 0.1           |
| (3,2848) | 1:84:A:ARG:HG2 | 1:84:A:ARG:HA   | 39       | 0.1           |
| (3,2809) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2  | 1        | 0.1           |
| (3,2809) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2  | 10       | 0.1           |
| (3,2809) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2  | 13       | 0.1           |
| (3,2761) | 1:90:A:GLU:HB3 | 1:91:A:ALA:H    | 18       | 0.1           |
| (3,2761) | 1:90:A:GLU:HB3 | 1:91:A:ALA:H    | 22       | 0.1           |
| (3,2761) | 1:90:A:GLU:HB3 | 1:91:A:ALA:H    | 23       | 0.1           |
| (3,2720) | 1:48:A:GLU:HA  | 1:41:A:THR:HG21 | 6        | 0.1           |
| (3,2720) | 1:48:A:GLU:HA  | 1:41:A:THR:HG22 | 6        | 0.1           |
| (3,2720) | 1:48:A:GLU:HA  | 1:41:A:THR:HG23 | 6        | 0.1           |
| (3,2720) | 1:48:A:GLU:HA  | 1:41:A:THR:HG21 | 9        | 0.1           |
| (3,2720) | 1:48:A:GLU:HA  | 1:41:A:THR:HG22 | 9        | 0.1           |
| (3,2720) | 1:48:A:GLU:HA  | 1:41:A:THR:HG23 | 9        | 0.1           |
| (3,2720) | 1:48:A:GLU:HA  | 1:41:A:THR:HG21 | 20       | 0.1           |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,2720) | 1:48:A:GLU:HA  | 1:41:A:THR:HG22 | 20       | 0.1           |
| (3,2720) | 1:48:A:GLU:HA  | 1:41:A:THR:HG23 | 20       | 0.1           |
| (3,2719) | 1:48:A:GLU:HA  | 1:49:A:LEU:HG   | 8        | 0.1           |
| (3,2719) | 1:48:A:GLU:HA  | 1:49:A:LEU:HG   | 27       | 0.1           |
| (3,2703) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA   | 18       | 0.1           |
| (3,2703) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA   | 29       | 0.1           |
| (3,2703) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA   | 37       | 0.1           |
| (3,2690) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 31       | 0.1           |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 2        | 0.1           |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 2        | 0.1           |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 2        | 0.1           |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 12       | 0.1           |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 12       | 0.1           |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 12       | 0.1           |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 29       | 0.1           |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 29       | 0.1           |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 29       | 0.1           |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 34       | 0.1           |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 34       | 0.1           |
| (3,2667) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 34       | 0.1           |
| (3,2653) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 4        | 0.1           |
| (3,2653) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 12       | 0.1           |
| (3,2653) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 31       | 0.1           |
| (3,2653) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 32       | 0.1           |
| (3,2653) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 34       | 0.1           |
| (3,2653) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 38       | 0.1           |
| (3,2650) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3   | 23       | 0.1           |
| (3,2650) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3   | 33       | 0.1           |
| (3,2650) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3   | 34       | 0.1           |
| (3,2650) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3   | 40       | 0.1           |
| (3,2613) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 3        | 0.1           |
| (3,2613) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 5        | 0.1           |
| (3,2613) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 12       | 0.1           |
| (3,2612) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 3        | 0.1           |
| (3,2612) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 5        | 0.1           |
| (3,2612) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 12       | 0.1           |
| (3,2554) | 1:92:A:ARG:HA  | 1:83:A:ALA:H    | 15       | 0.1           |
| (3,2548) | 1:70:A:ASN:HA  | 1:24:A:HIS:HA   | 33       | 0.1           |
| (3,2541) | 1:73:A:PRO:HG3 | 1:73:A:PRO:HA   | 28       | 0.1           |
| (3,2541) | 1:73:A:PRO:HG3 | 1:73:A:PRO:HA   | 32       | 0.1           |
| (3,2434) | 1:82:A:ILE:HB  | 1:41:A:THR:H    | 20       | 0.1           |
| (3,2434) | 1:82:A:ILE:HB  | 1:41:A:THR:H    | 39       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2419) | 1:10:A:ILE:HB   | 1:9:A:PRO:HA    | 8        | 0.1           |
| (3,2419) | 1:10:A:ILE:HB   | 1:9:A:PRO:HA    | 14       | 0.1           |
| (3,2419) | 1:10:A:ILE:HB   | 1:9:A:PRO:HA    | 28       | 0.1           |
| (3,2419) | 1:10:A:ILE:HB   | 1:9:A:PRO:HA    | 29       | 0.1           |
| (3,2419) | 1:10:A:ILE:HB   | 1:9:A:PRO:HA    | 31       | 0.1           |
| (3,2406) | 1:66:A:MET:HE1  | 1:42:A:TRP:H    | 21       | 0.1           |
| (3,2406) | 1:66:A:MET:HE2  | 1:42:A:TRP:H    | 21       | 0.1           |
| (3,2406) | 1:66:A:MET:HE3  | 1:42:A:TRP:H    | 21       | 0.1           |
| (3,2405) | 1:66:A:MET:HE1  | 1:29:A:PHE:HZ   | 28       | 0.1           |
| (3,2405) | 1:66:A:MET:HE2  | 1:29:A:PHE:HZ   | 28       | 0.1           |
| (3,2405) | 1:66:A:MET:HE3  | 1:29:A:PHE:HZ   | 28       | 0.1           |
| (3,2405) | 1:66:A:MET:HE1  | 1:29:A:PHE:HZ   | 29       | 0.1           |
| (3,2405) | 1:66:A:MET:HE2  | 1:29:A:PHE:HZ   | 29       | 0.1           |
| (3,2405) | 1:66:A:MET:HE3  | 1:29:A:PHE:HZ   | 29       | 0.1           |
| (3,2334) | 1:26:A:SER:HA   | 1:68:A:ILE:HG21 | 24       | 0.1           |
| (3,2334) | 1:26:A:SER:HA   | 1:68:A:ILE:HG22 | 24       | 0.1           |
| (3,2334) | 1:26:A:SER:HA   | 1:68:A:ILE:HG23 | 24       | 0.1           |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG21 | 4        | 0.1           |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG22 | 4        | 0.1           |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG23 | 4        | 0.1           |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG21 | 25       | 0.1           |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG22 | 25       | 0.1           |
| (3,2268) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG23 | 25       | 0.1           |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD11 | 23       | 0.1           |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD12 | 23       | 0.1           |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD13 | 23       | 0.1           |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD11 | 29       | 0.1           |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD12 | 29       | 0.1           |
| (3,2168) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD13 | 29       | 0.1           |
| (3,2148) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 4        | 0.1           |
| (3,2148) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 17       | 0.1           |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1  | 13       | 0.1           |
| (3,2082) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2  | 13       | 0.1           |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1  | 13       | 0.1           |
| (3,2082) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2  | 13       | 0.1           |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1  | 13       | 0.1           |
| (3,2082) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2  | 13       | 0.1           |
| (3,2075) | 1:97:A:LEU:HB2  | 1:19:A:ILE:HB   | 1        | 0.1           |
| (3,2075) | 1:97:A:LEU:HB2  | 1:19:A:ILE:HB   | 10       | 0.1           |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD11 | 19       | 0.1           |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD12 | 19       | 0.1           |
| (3,2071) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD13 | 19       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD11 | 19       | 0.1           |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD12 | 19       | 0.1           |
| (3,2071) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD13 | 19       | 0.1           |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD11 | 19       | 0.1           |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD12 | 19       | 0.1           |
| (3,2071) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD13 | 19       | 0.1           |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1  | 4        | 0.1           |
| (3,2046) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2  | 4        | 0.1           |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1  | 4        | 0.1           |
| (3,2046) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2  | 4        | 0.1           |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1  | 4        | 0.1           |
| (3,2046) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2  | 4        | 0.1           |
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3  | 19       | 0.1           |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3  | 19       | 0.1           |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3  | 19       | 0.1           |
| (3,2026) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3  | 26       | 0.1           |
| (3,2026) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3  | 26       | 0.1           |
| (3,2026) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3  | 26       | 0.1           |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 8        | 0.1           |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 10       | 0.1           |
| (3,2010) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 13       | 0.1           |
| (3,2007) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 26       | 0.1           |
| (3,2007) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 26       | 0.1           |
| (3,2007) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 26       | 0.1           |
| (3,1993) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 17       | 0.1           |
| (3,1993) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 17       | 0.1           |
| (3,1993) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 17       | 0.1           |
| (3,1993) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 22       | 0.1           |
| (3,1993) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 22       | 0.1           |
| (3,1993) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 22       | 0.1           |
| (3,1981) | 1:16:A:ILE:HG21 | 1:30:A:GLU:H    | 11       | 0.1           |
| (3,1981) | 1:16:A:ILE:HG22 | 1:30:A:GLU:H    | 11       | 0.1           |
| (3,1981) | 1:16:A:ILE:HG23 | 1:30:A:GLU:H    | 11       | 0.1           |
| (3,1965) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 21       | 0.1           |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H    | 3        | 0.1           |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H    | 3        | 0.1           |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H    | 3        | 0.1           |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H    | 6        | 0.1           |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H    | 6        | 0.1           |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H    | 6        | 0.1           |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H    | 16       | 0.1           |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H    | 16       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H    | 16       | 0.1           |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H    | 31       | 0.1           |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H    | 31       | 0.1           |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H    | 31       | 0.1           |
| (3,1922) | 1:50:A:THR:HG21 | 1:51:A:GLU:H    | 40       | 0.1           |
| (3,1922) | 1:50:A:THR:HG22 | 1:51:A:GLU:H    | 40       | 0.1           |
| (3,1922) | 1:50:A:THR:HG23 | 1:51:A:GLU:H    | 40       | 0.1           |
| (3,1912) | 1:10:A:ILE:HD11 | 1:85:A:LEU:HD11 | 14       | 0.1           |
| (3,1912) | 1:10:A:ILE:HD11 | 1:85:A:LEU:HD12 | 14       | 0.1           |
| (3,1912) | 1:10:A:ILE:HD11 | 1:85:A:LEU:HD13 | 14       | 0.1           |
| (3,1912) | 1:10:A:ILE:HD12 | 1:85:A:LEU:HD11 | 14       | 0.1           |
| (3,1912) | 1:10:A:ILE:HD12 | 1:85:A:LEU:HD12 | 14       | 0.1           |
| (3,1912) | 1:10:A:ILE:HD12 | 1:85:A:LEU:HD13 | 14       | 0.1           |
| (3,1912) | 1:10:A:ILE:HD13 | 1:85:A:LEU:HD11 | 14       | 0.1           |
| (3,1912) | 1:10:A:ILE:HD13 | 1:85:A:LEU:HD12 | 14       | 0.1           |
| (3,1912) | 1:10:A:ILE:HD13 | 1:85:A:LEU:HD13 | 14       | 0.1           |
| (3,1906) | 1:66:A:MET:HE1  | 1:79:A:TYR:HA   | 19       | 0.1           |
| (3,1906) | 1:66:A:MET:HE2  | 1:79:A:TYR:HA   | 19       | 0.1           |
| (3,1906) | 1:66:A:MET:HE3  | 1:79:A:TYR:HA   | 19       | 0.1           |
| (3,1906) | 1:66:A:MET:HE1  | 1:79:A:TYR:HA   | 28       | 0.1           |
| (3,1906) | 1:66:A:MET:HE2  | 1:79:A:TYR:HA   | 28       | 0.1           |
| (3,1906) | 1:66:A:MET:HE3  | 1:79:A:TYR:HA   | 28       | 0.1           |
| (3,1899) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3  | 3        | 0.1           |
| (3,1899) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3  | 3        | 0.1           |
| (3,1899) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3  | 3        | 0.1           |
| (3,1899) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3  | 9        | 0.1           |
| (3,1899) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3  | 9        | 0.1           |
| (3,1899) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3  | 9        | 0.1           |
| (3,1899) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3  | 17       | 0.1           |
| (3,1899) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3  | 17       | 0.1           |
| (3,1899) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3  | 17       | 0.1           |
| (3,1899) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3  | 32       | 0.1           |
| (3,1899) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3  | 32       | 0.1           |
| (3,1899) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3  | 32       | 0.1           |
| (3,1899) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3  | 35       | 0.1           |
| (3,1899) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3  | 35       | 0.1           |
| (3,1899) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3  | 35       | 0.1           |
| (3,1866) | 1:7:A:ALA:HB1   | 1:8:A:GLU:H     | 31       | 0.1           |
| (3,1866) | 1:7:A:ALA:HB2   | 1:8:A:GLU:H     | 31       | 0.1           |
| (3,1866) | 1:7:A:ALA:HB3   | 1:8:A:GLU:H     | 31       | 0.1           |
| (3,1864) | 1:7:A:ALA:HB1   | 1:88:A:ARG:HA   | 23       | 0.1           |
| (3,1864) | 1:7:A:ALA:HB2   | 1:88:A:ARG:HA   | 23       | 0.1           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (3,1864) | 1:7:A:ALA:HB3    | 1:88:A:ARG:HA   | 23       | 0.1           |
| (3,1856) | 1:27:A:ALA:HB1   | 1:28:A:THR:H    | 5        | 0.1           |
| (3,1856) | 1:27:A:ALA:HB2   | 1:28:A:THR:H    | 5        | 0.1           |
| (3,1856) | 1:27:A:ALA:HB3   | 1:28:A:THR:H    | 5        | 0.1           |
| (3,1850) | 1:27:A:ALA:HB1   | 1:19:A:ILE:HG21 | 14       | 0.1           |
| (3,1850) | 1:27:A:ALA:HB1   | 1:19:A:ILE:HG22 | 14       | 0.1           |
| (3,1850) | 1:27:A:ALA:HB1   | 1:19:A:ILE:HG23 | 14       | 0.1           |
| (3,1850) | 1:27:A:ALA:HB2   | 1:19:A:ILE:HG21 | 14       | 0.1           |
| (3,1850) | 1:27:A:ALA:HB2   | 1:19:A:ILE:HG22 | 14       | 0.1           |
| (3,1850) | 1:27:A:ALA:HB2   | 1:19:A:ILE:HG23 | 14       | 0.1           |
| (3,1850) | 1:27:A:ALA:HB3   | 1:19:A:ILE:HG21 | 14       | 0.1           |
| (3,1850) | 1:27:A:ALA:HB3   | 1:19:A:ILE:HG22 | 14       | 0.1           |
| (3,1850) | 1:27:A:ALA:HB3   | 1:19:A:ILE:HG23 | 14       | 0.1           |
| (3,1728) | 1:38:A:ALA:HB1   | 1:83:A:ALA:HA   | 4        | 0.1           |
| (3,1728) | 1:38:A:ALA:HB2   | 1:83:A:ALA:HA   | 4        | 0.1           |
| (3,1728) | 1:38:A:ALA:HB3   | 1:83:A:ALA:HA   | 4        | 0.1           |
| (3,1700) | 1:101:A:LEU:HD21 | 1:101:A:LEU:HB3 | 15       | 0.1           |
| (3,1700) | 1:101:A:LEU:HD22 | 1:101:A:LEU:HB3 | 15       | 0.1           |
| (3,1700) | 1:101:A:LEU:HD23 | 1:101:A:LEU:HB3 | 15       | 0.1           |
| (3,1700) | 1:101:A:LEU:HD21 | 1:101:A:LEU:HB3 | 26       | 0.1           |
| (3,1700) | 1:101:A:LEU:HD22 | 1:101:A:LEU:HB3 | 26       | 0.1           |
| (3,1700) | 1:101:A:LEU:HD23 | 1:101:A:LEU:HB3 | 26       | 0.1           |
| (3,1689) | 1:97:A:LEU:HD11  | 1:71:A:VAL:HG21 | 4        | 0.1           |
| (3,1689) | 1:97:A:LEU:HD11  | 1:71:A:VAL:HG22 | 4        | 0.1           |
| (3,1689) | 1:97:A:LEU:HD11  | 1:71:A:VAL:HG23 | 4        | 0.1           |
| (3,1689) | 1:97:A:LEU:HD12  | 1:71:A:VAL:HG21 | 4        | 0.1           |
| (3,1689) | 1:97:A:LEU:HD12  | 1:71:A:VAL:HG22 | 4        | 0.1           |
| (3,1689) | 1:97:A:LEU:HD12  | 1:71:A:VAL:HG23 | 4        | 0.1           |
| (3,1689) | 1:97:A:LEU:HD13  | 1:71:A:VAL:HG21 | 4        | 0.1           |
| (3,1689) | 1:97:A:LEU:HD13  | 1:71:A:VAL:HG22 | 4        | 0.1           |
| (3,1689) | 1:97:A:LEU:HD13  | 1:71:A:VAL:HG23 | 4        | 0.1           |
| (3,1689) | 1:97:A:LEU:HD11  | 1:71:A:VAL:HG21 | 16       | 0.1           |
| (3,1689) | 1:97:A:LEU:HD11  | 1:71:A:VAL:HG22 | 16       | 0.1           |
| (3,1689) | 1:97:A:LEU:HD11  | 1:71:A:VAL:HG23 | 16       | 0.1           |
| (3,1689) | 1:97:A:LEU:HD12  | 1:71:A:VAL:HG21 | 16       | 0.1           |
| (3,1689) | 1:97:A:LEU:HD12  | 1:71:A:VAL:HG22 | 16       | 0.1           |
| (3,1689) | 1:97:A:LEU:HD12  | 1:71:A:VAL:HG23 | 16       | 0.1           |
| (3,1689) | 1:97:A:LEU:HD13  | 1:71:A:VAL:HG21 | 16       | 0.1           |
| (3,1689) | 1:97:A:LEU:HD13  | 1:71:A:VAL:HG22 | 16       | 0.1           |
| (3,1689) | 1:97:A:LEU:HD13  | 1:71:A:VAL:HG23 | 16       | 0.1           |
| (3,1683) | 1:85:A:LEU:HD11  | 1:35:A:PHE:HD1  | 14       | 0.1           |
| (3,1683) | 1:85:A:LEU:HD11  | 1:35:A:PHE:HD2  | 14       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1683) | 1:85:A:LEU:HD12 | 1:35:A:PHE:HD1  | 14       | 0.1           |
| (3,1683) | 1:85:A:LEU:HD12 | 1:35:A:PHE:HD2  | 14       | 0.1           |
| (3,1683) | 1:85:A:LEU:HD13 | 1:35:A:PHE:HD1  | 14       | 0.1           |
| (3,1683) | 1:85:A:LEU:HD13 | 1:35:A:PHE:HD2  | 14       | 0.1           |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 34       | 0.1           |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 34       | 0.1           |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 34       | 0.1           |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 38       | 0.1           |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 38       | 0.1           |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 38       | 0.1           |
| (3,1682) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 40       | 0.1           |
| (3,1682) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 40       | 0.1           |
| (3,1682) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 40       | 0.1           |
| (3,1654) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 2        | 0.1           |
| (3,1654) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 2        | 0.1           |
| (3,1654) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 2        | 0.1           |
| (3,1654) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 2        | 0.1           |
| (3,1654) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 2        | 0.1           |
| (3,1654) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 2        | 0.1           |
| (3,1654) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 2        | 0.1           |
| (3,1654) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 2        | 0.1           |
| (3,1654) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 2        | 0.1           |
| (3,1654) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 38       | 0.1           |
| (3,1654) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 38       | 0.1           |
| (3,1654) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 38       | 0.1           |
| (3,1654) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 38       | 0.1           |
| (3,1654) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 38       | 0.1           |
| (3,1654) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 38       | 0.1           |
| (3,1654) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 38       | 0.1           |
| (3,1654) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 38       | 0.1           |
| (3,1654) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 38       | 0.1           |
| (3,1626) | 1:82:A:ILE:HD11 | 1:83:A:ALA:H    | 11       | 0.1           |
| (3,1626) | 1:82:A:ILE:HD12 | 1:83:A:ALA:H    | 11       | 0.1           |
| (3,1626) | 1:82:A:ILE:HD13 | 1:83:A:ALA:H    | 11       | 0.1           |
| (3,1626) | 1:82:A:ILE:HD11 | 1:83:A:ALA:H    | 28       | 0.1           |
| (3,1626) | 1:82:A:ILE:HD12 | 1:83:A:ALA:H    | 28       | 0.1           |
| (3,1626) | 1:82:A:ILE:HD13 | 1:83:A:ALA:H    | 28       | 0.1           |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1  | 5        | 0.1           |
| (3,1605) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2  | 5        | 0.1           |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1  | 5        | 0.1           |
| (3,1605) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2  | 5        | 0.1           |
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1  | 5        | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1605) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2  | 5        | 0.1           |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 10       | 0.1           |
| (3,1604) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 10       | 0.1           |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 10       | 0.1           |
| (3,1604) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 10       | 0.1           |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 10       | 0.1           |
| (3,1604) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 10       | 0.1           |
| (3,1554) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA    | 19       | 0.1           |
| (3,1554) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA    | 19       | 0.1           |
| (3,1554) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA    | 19       | 0.1           |
| (3,1554) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA    | 30       | 0.1           |
| (3,1554) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA    | 30       | 0.1           |
| (3,1554) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA    | 30       | 0.1           |
| (3,1554) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA    | 35       | 0.1           |
| (3,1554) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA    | 35       | 0.1           |
| (3,1554) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA    | 35       | 0.1           |
| (3,1517) | 1:66:A:MET:HE1  | 1:29:A:PHE:H    | 27       | 0.1           |
| (3,1517) | 1:66:A:MET:HE2  | 1:29:A:PHE:H    | 27       | 0.1           |
| (3,1517) | 1:66:A:MET:HE3  | 1:29:A:PHE:H    | 27       | 0.1           |
| (3,1517) | 1:66:A:MET:HE1  | 1:29:A:PHE:H    | 31       | 0.1           |
| (3,1517) | 1:66:A:MET:HE2  | 1:29:A:PHE:H    | 31       | 0.1           |
| (3,1517) | 1:66:A:MET:HE3  | 1:29:A:PHE:H    | 31       | 0.1           |
| (3,1514) | 1:66:A:MET:HE1  | 1:42:A:TRP:HE1  | 3        | 0.1           |
| (3,1514) | 1:66:A:MET:HE2  | 1:42:A:TRP:HE1  | 3        | 0.1           |
| (3,1514) | 1:66:A:MET:HE3  | 1:42:A:TRP:HE1  | 3        | 0.1           |
| (3,1514) | 1:66:A:MET:HE1  | 1:42:A:TRP:HE1  | 37       | 0.1           |
| (3,1514) | 1:66:A:MET:HE2  | 1:42:A:TRP:HE1  | 37       | 0.1           |
| (3,1514) | 1:66:A:MET:HE3  | 1:42:A:TRP:HE1  | 37       | 0.1           |
| (3,1512) | 1:66:A:MET:HE1  | 1:42:A:TRP:HZ3  | 2        | 0.1           |
| (3,1512) | 1:66:A:MET:HE2  | 1:42:A:TRP:HZ3  | 2        | 0.1           |
| (3,1512) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3  | 2        | 0.1           |
| (3,1512) | 1:66:A:MET:HE1  | 1:42:A:TRP:HZ3  | 24       | 0.1           |
| (3,1512) | 1:66:A:MET:HE2  | 1:42:A:TRP:HZ3  | 24       | 0.1           |
| (3,1512) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3  | 24       | 0.1           |
| (3,1511) | 1:66:A:MET:HE1  | 1:42:A:TRP:HB2  | 13       | 0.1           |
| (3,1511) | 1:66:A:MET:HE2  | 1:42:A:TRP:HB2  | 13       | 0.1           |
| (3,1511) | 1:66:A:MET:HE3  | 1:42:A:TRP:HB2  | 13       | 0.1           |
| (3,1506) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD11 | 14       | 0.1           |
| (3,1506) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD12 | 14       | 0.1           |
| (3,1506) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD13 | 14       | 0.1           |
| (3,1506) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD11 | 14       | 0.1           |
| (3,1506) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD12 | 14       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1506) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD13 | 14       | 0.1           |
| (3,1506) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD11 | 14       | 0.1           |
| (3,1506) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD12 | 14       | 0.1           |
| (3,1506) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD13 | 14       | 0.1           |
| (3,1506) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD11 | 26       | 0.1           |
| (3,1506) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD12 | 26       | 0.1           |
| (3,1506) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD13 | 26       | 0.1           |
| (3,1506) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD11 | 26       | 0.1           |
| (3,1506) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD12 | 26       | 0.1           |
| (3,1506) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD13 | 26       | 0.1           |
| (3,1506) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD11 | 26       | 0.1           |
| (3,1506) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD12 | 26       | 0.1           |
| (3,1506) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD13 | 26       | 0.1           |
| (3,1498) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 5        | 0.1           |
| (3,1498) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 5        | 0.1           |
| (3,1498) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 5        | 0.1           |
| (3,1498) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 25       | 0.1           |
| (3,1498) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 25       | 0.1           |
| (3,1498) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 25       | 0.1           |
| (3,1498) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 29       | 0.1           |
| (3,1498) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 29       | 0.1           |
| (3,1498) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 29       | 0.1           |
| (3,1488) | 1:81:A:VAL:HB   | 1:42:A:TRP:HE1  | 4        | 0.1           |
| (3,1488) | 1:81:A:VAL:HB   | 1:42:A:TRP:HE1  | 7        | 0.1           |
| (3,1488) | 1:81:A:VAL:HB   | 1:42:A:TRP:HE1  | 31       | 0.1           |
| (3,1477) | 1:78:A:VAL:HG11 | 1:94:A:THR:HB   | 28       | 0.1           |
| (3,1477) | 1:78:A:VAL:HG12 | 1:94:A:THR:HB   | 28       | 0.1           |
| (3,1477) | 1:78:A:VAL:HG13 | 1:94:A:THR:HB   | 28       | 0.1           |
| (3,1412) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HA  | 33       | 0.1           |
| (3,1412) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HA  | 33       | 0.1           |
| (3,1412) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HA  | 33       | 0.1           |
| (3,1388) | 1:91:A:ALA:HB1  | 1:83:A:ALA:HB1  | 7        | 0.1           |
| (3,1388) | 1:91:A:ALA:HB1  | 1:83:A:ALA:HB2  | 7        | 0.1           |
| (3,1388) | 1:91:A:ALA:HB1  | 1:83:A:ALA:HB3  | 7        | 0.1           |
| (3,1388) | 1:91:A:ALA:HB2  | 1:83:A:ALA:HB1  | 7        | 0.1           |
| (3,1388) | 1:91:A:ALA:HB2  | 1:83:A:ALA:HB2  | 7        | 0.1           |
| (3,1388) | 1:91:A:ALA:HB2  | 1:83:A:ALA:HB3  | 7        | 0.1           |
| (3,1388) | 1:91:A:ALA:HB3  | 1:83:A:ALA:HB1  | 7        | 0.1           |
| (3,1388) | 1:91:A:ALA:HB3  | 1:83:A:ALA:HB2  | 7        | 0.1           |
| (3,1388) | 1:91:A:ALA:HB3  | 1:83:A:ALA:HB3  | 7        | 0.1           |
| (3,1383) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB1  | 7        | 0.1           |
| (3,1383) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB2  | 7        | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1383) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB3  | 7        | 0.1           |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB1  | 7        | 0.1           |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB2  | 7        | 0.1           |
| (3,1383) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB3  | 7        | 0.1           |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB1  | 7        | 0.1           |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB2  | 7        | 0.1           |
| (3,1383) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB3  | 7        | 0.1           |
| (3,1372) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 28       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 1        | 0.1           |
| (3,1361) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 1        | 0.1           |
| (3,1361) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 1        | 0.1           |
| (3,1361) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 3        | 0.1           |
| (3,1361) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 3        | 0.1           |
| (3,1361) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 3        | 0.1           |
| (3,1361) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 4        | 0.1           |
| (3,1361) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 4        | 0.1           |
| (3,1361) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 4        | 0.1           |
| (3,1361) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 6        | 0.1           |
| (3,1361) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 6        | 0.1           |
| (3,1361) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 6        | 0.1           |
| (3,1361) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 11       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 11       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 11       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 12       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 12       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 12       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 13       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 13       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 13       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 14       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 14       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 14       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 20       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 20       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 20       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 23       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 23       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 23       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 25       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 25       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 25       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 30       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1361) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 30       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 30       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 31       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 31       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 31       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 34       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 34       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 34       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 35       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 35       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 35       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 36       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 36       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 36       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 40       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 40       | 0.1           |
| (3,1361) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 40       | 0.1           |
| (3,1352) | 1:16:A:ILE:HD11 | 1:95:A:ALA:H    | 5        | 0.1           |
| (3,1352) | 1:16:A:ILE:HD12 | 1:95:A:ALA:H    | 5        | 0.1           |
| (3,1352) | 1:16:A:ILE:HD13 | 1:95:A:ALA:H    | 5        | 0.1           |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 3        | 0.1           |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 10       | 0.1           |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 27       | 0.1           |
| (3,1299) | 1:40:A:VAL:HB   | 1:41:A:THR:H    | 39       | 0.1           |
| (3,1270) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 28       | 0.1           |
| (3,1270) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 28       | 0.1           |
| (3,1270) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 28       | 0.1           |
| (3,1269) | 1:94:A:THR:HG21 | 1:95:A:ALA:H    | 28       | 0.1           |
| (3,1269) | 1:94:A:THR:HG22 | 1:95:A:ALA:H    | 28       | 0.1           |
| (3,1269) | 1:94:A:THR:HG23 | 1:95:A:ALA:H    | 28       | 0.1           |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 4        | 0.1           |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 4        | 0.1           |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 4        | 0.1           |
| (3,1268) | 1:94:A:THR:HG21 | 1:93:A:SER:HA   | 9        | 0.1           |
| (3,1268) | 1:94:A:THR:HG22 | 1:93:A:SER:HA   | 9        | 0.1           |
| (3,1268) | 1:94:A:THR:HG23 | 1:93:A:SER:HA   | 9        | 0.1           |
| (3,1265) | 1:67:A:THR:HG21 | 1:56:A:ASN:H    | 13       | 0.1           |
| (3,1265) | 1:67:A:THR:HG22 | 1:56:A:ASN:H    | 13       | 0.1           |
| (3,1265) | 1:67:A:THR:HG23 | 1:56:A:ASN:H    | 13       | 0.1           |
| (3,1265) | 1:67:A:THR:HG21 | 1:56:A:ASN:H    | 31       | 0.1           |
| (3,1265) | 1:67:A:THR:HG22 | 1:56:A:ASN:H    | 31       | 0.1           |
| (3,1265) | 1:67:A:THR:HG23 | 1:56:A:ASN:H    | 31       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,1265) | 1:67:A:THR:HG21 | 1:56:A:ASN:H    | 35       | 0.1           |
| (3,1265) | 1:67:A:THR:HG22 | 1:56:A:ASN:H    | 35       | 0.1           |
| (3,1265) | 1:67:A:THR:HG23 | 1:56:A:ASN:H    | 35       | 0.1           |
| (3,1243) | 1:13:A:THR:HG21 | 1:34:A:SER:H    | 8        | 0.1           |
| (3,1243) | 1:13:A:THR:HG22 | 1:34:A:SER:H    | 8        | 0.1           |
| (3,1243) | 1:13:A:THR:HG23 | 1:34:A:SER:H    | 8        | 0.1           |
| (3,1243) | 1:13:A:THR:HG21 | 1:34:A:SER:H    | 11       | 0.1           |
| (3,1243) | 1:13:A:THR:HG22 | 1:34:A:SER:H    | 11       | 0.1           |
| (3,1243) | 1:13:A:THR:HG23 | 1:34:A:SER:H    | 11       | 0.1           |
| (3,1243) | 1:13:A:THR:HG21 | 1:34:A:SER:H    | 35       | 0.1           |
| (3,1243) | 1:13:A:THR:HG22 | 1:34:A:SER:H    | 35       | 0.1           |
| (3,1243) | 1:13:A:THR:HG23 | 1:34:A:SER:H    | 35       | 0.1           |
| (3,1240) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3  | 33       | 0.1           |
| (3,1240) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3  | 33       | 0.1           |
| (3,1240) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3  | 33       | 0.1           |
| (3,1230) | 1:101:A:LEU:H   | 1:22:A:SER:HA   | 12       | 0.1           |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 12       | 0.1           |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 12       | 0.1           |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 12       | 0.1           |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 14       | 0.1           |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 14       | 0.1           |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 14       | 0.1           |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 18       | 0.1           |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 18       | 0.1           |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 18       | 0.1           |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD21 | 34       | 0.1           |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD22 | 34       | 0.1           |
| (3,1226) | 1:97:A:LEU:H    | 1:97:A:LEU:HD23 | 34       | 0.1           |
| (3,1221) | 1:69:A:HIS:H    | 1:56:A:ASN:H    | 10       | 0.1           |
| (3,1217) | 1:66:A:MET:H    | 1:28:A:THR:HA   | 15       | 0.1           |
| (3,1217) | 1:66:A:MET:H    | 1:28:A:THR:HA   | 28       | 0.1           |
| (3,1212) | 1:56:A:ASN:H    | 1:66:A:MET:HG2  | 8        | 0.1           |
| (3,1212) | 1:56:A:ASN:H    | 1:66:A:MET:HG2  | 14       | 0.1           |
| (3,1212) | 1:56:A:ASN:H    | 1:66:A:MET:HG2  | 20       | 0.1           |
| (3,1208) | 1:42:A:TRP:H    | 1:57:A:PHE:HE1  | 24       | 0.1           |
| (3,1208) | 1:42:A:TRP:H    | 1:57:A:PHE:HE2  | 24       | 0.1           |
| (3,1206) | 1:41:A:THR:H    | 1:83:A:ALA:HA   | 12       | 0.1           |
| (3,1178) | 1:91:A:ALA:H    | 1:84:A:ARG:HA   | 14       | 0.1           |
| (3,1152) | 1:54:A:LYS:H    | 1:53:A:GLN:HG3  | 14       | 0.1           |
| (3,1152) | 1:54:A:LYS:H    | 1:53:A:GLN:HG3  | 26       | 0.1           |
| (3,1152) | 1:54:A:LYS:H    | 1:53:A:GLN:HG3  | 29       | 0.1           |
| (3,1140) | 1:100:A:GLU:H   | 1:101:A:LEU:H   | 22       | 0.1           |

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| Key      | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|----------|--------------|-----------------|----------|---------------|
| (3,1131) | 1:40:A:VAL:H | 1:83:A:ALA:HB1  | 16       | 0.1           |
| (3,1131) | 1:40:A:VAL:H | 1:83:A:ALA:HB2  | 16       | 0.1           |
| (3,1131) | 1:40:A:VAL:H | 1:83:A:ALA:HB3  | 16       | 0.1           |
| (3,1055) | 1:33:A:VAL:H | 1:62:A:ARG:HB2  | 17       | 0.1           |
| (3,1051) | 1:26:A:SER:H | 1:25:A:GLN:HG2  | 7        | 0.1           |
| (3,1019) | 1:48:A:GLU:H | 1:48:A:GLU:HG3  | 14       | 0.1           |
| (3,1019) | 1:48:A:GLU:H | 1:48:A:GLU:HG3  | 30       | 0.1           |
| (3,998)  | 1:79:A:TYR:H | 1:94:A:THR:HG21 | 6        | 0.1           |
| (3,998)  | 1:79:A:TYR:H | 1:94:A:THR:HG22 | 6        | 0.1           |
| (3,998)  | 1:79:A:TYR:H | 1:94:A:THR:HG23 | 6        | 0.1           |
| (3,998)  | 1:79:A:TYR:H | 1:94:A:THR:HG21 | 18       | 0.1           |
| (3,998)  | 1:79:A:TYR:H | 1:94:A:THR:HG22 | 18       | 0.1           |
| (3,998)  | 1:79:A:TYR:H | 1:94:A:THR:HG23 | 18       | 0.1           |
| (3,998)  | 1:79:A:TYR:H | 1:94:A:THR:HG21 | 20       | 0.1           |
| (3,998)  | 1:79:A:TYR:H | 1:94:A:THR:HG22 | 20       | 0.1           |
| (3,998)  | 1:79:A:TYR:H | 1:94:A:THR:HG23 | 20       | 0.1           |
| (3,988)  | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 7        | 0.1           |
| (3,988)  | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 13       | 0.1           |
| (3,988)  | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 19       | 0.1           |
| (3,949)  | 1:34:A:SER:H | 1:33:A:VAL:HG21 | 20       | 0.1           |
| (3,949)  | 1:34:A:SER:H | 1:33:A:VAL:HG22 | 20       | 0.1           |
| (3,949)  | 1:34:A:SER:H | 1:33:A:VAL:HG23 | 20       | 0.1           |
| (3,942)  | 1:34:A:SER:H | 1:12:A:PHE:HA   | 7        | 0.1           |
| (3,942)  | 1:34:A:SER:H | 1:12:A:PHE:HA   | 9        | 0.1           |
| (3,942)  | 1:34:A:SER:H | 1:12:A:PHE:HA   | 14       | 0.1           |
| (3,934)  | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 22       | 0.1           |
| (3,934)  | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 22       | 0.1           |
| (3,934)  | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 22       | 0.1           |
| (3,934)  | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 33       | 0.1           |
| (3,934)  | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 33       | 0.1           |
| (3,934)  | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 33       | 0.1           |
| (3,934)  | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 37       | 0.1           |
| (3,934)  | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 37       | 0.1           |
| (3,934)  | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 37       | 0.1           |
| (3,934)  | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 38       | 0.1           |
| (3,934)  | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 38       | 0.1           |
| (3,934)  | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 38       | 0.1           |
| (3,916)  | 1:37:A:ASP:H | 1:37:A:ASP:HA   | 2        | 0.1           |
| (3,900)  | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 2        | 0.1           |
| (3,900)  | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 16       | 0.1           |
| (3,900)  | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 33       | 0.1           |
| (3,900)  | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 40       | 0.1           |

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| Key     | Atom-1       | Atom-2         | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (3,890) | 1:80:A:SER:H | 1:79:A:TYR:HB2 | 1        | 0.1           |
| (3,890) | 1:80:A:SER:H | 1:79:A:TYR:HB2 | 3        | 0.1           |
| (3,890) | 1:80:A:SER:H | 1:79:A:TYR:HB2 | 4        | 0.1           |
| (3,890) | 1:80:A:SER:H | 1:79:A:TYR:HB2 | 9        | 0.1           |
| (3,890) | 1:80:A:SER:H | 1:79:A:TYR:HB2 | 23       | 0.1           |
| (3,890) | 1:80:A:SER:H | 1:79:A:TYR:HB2 | 24       | 0.1           |
| (3,890) | 1:80:A:SER:H | 1:79:A:TYR:HB2 | 30       | 0.1           |
| (3,890) | 1:80:A:SER:H | 1:79:A:TYR:HB2 | 39       | 0.1           |
| (3,890) | 1:80:A:SER:H | 1:79:A:TYR:HB2 | 40       | 0.1           |
| (3,889) | 1:80:A:SER:H | 1:43:A:TYR:HB3 | 33       | 0.1           |
| (3,875) | 1:8:A:GLU:H  | 1:7:A:ALA:HB1  | 31       | 0.1           |
| (3,875) | 1:8:A:GLU:H  | 1:7:A:ALA:HB2  | 31       | 0.1           |
| (3,875) | 1:8:A:GLU:H  | 1:7:A:ALA:HB3  | 31       | 0.1           |
| (3,864) | 1:86:A:GLU:H | 1:86:A:GLU:HG3 | 9        | 0.1           |
| (3,863) | 1:86:A:GLU:H | 1:85:A:LEU:HB3 | 21       | 0.1           |
| (3,863) | 1:86:A:GLU:H | 1:85:A:LEU:HB3 | 36       | 0.1           |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1 | 39       | 0.1           |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2 | 39       | 0.1           |
| (3,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3 | 39       | 0.1           |
| (3,813) | 1:25:A:GLN:H | 1:25:A:GLN:HG3 | 19       | 0.1           |
| (3,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB  | 37       | 0.1           |
| (3,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB  | 38       | 0.1           |
| (3,742) | 1:76:A:GLU:H | 1:77:A:GLY:H   | 6        | 0.1           |
| (3,742) | 1:76:A:GLU:H | 1:77:A:GLY:H   | 9        | 0.1           |
| (3,742) | 1:76:A:GLU:H | 1:77:A:GLY:H   | 13       | 0.1           |
| (3,742) | 1:76:A:GLU:H | 1:77:A:GLY:H   | 19       | 0.1           |
| (3,742) | 1:76:A:GLU:H | 1:77:A:GLY:H   | 37       | 0.1           |
| (3,726) | 1:49:A:LEU:H | 1:48:A:GLU:HG3 | 2        | 0.1           |
| (3,726) | 1:49:A:LEU:H | 1:48:A:GLU:HG3 | 7        | 0.1           |
| (3,726) | 1:49:A:LEU:H | 1:48:A:GLU:HG3 | 11       | 0.1           |
| (3,709) | 1:16:A:ILE:H | 1:31:A:CYS:HB2 | 1        | 0.1           |
| (3,709) | 1:16:A:ILE:H | 1:31:A:CYS:HB2 | 6        | 0.1           |
| (3,666) | 1:72:A:THR:H | 1:72:A:THR:HB  | 8        | 0.1           |
| (3,666) | 1:72:A:THR:H | 1:72:A:THR:HB  | 9        | 0.1           |
| (3,666) | 1:72:A:THR:H | 1:72:A:THR:HB  | 20       | 0.1           |
| (3,666) | 1:72:A:THR:H | 1:72:A:THR:HB  | 30       | 0.1           |
| (3,666) | 1:72:A:THR:H | 1:72:A:THR:HB  | 33       | 0.1           |
| (3,666) | 1:72:A:THR:H | 1:72:A:THR:HB  | 34       | 0.1           |
| (3,666) | 1:72:A:THR:H | 1:72:A:THR:HB  | 35       | 0.1           |
| (3,661) | 1:7:A:ALA:H  | 1:6:A:THR:HA   | 3        | 0.1           |
| (3,661) | 1:7:A:ALA:H  | 1:6:A:THR:HA   | 13       | 0.1           |
| (3,661) | 1:7:A:ALA:H  | 1:6:A:THR:HA   | 29       | 0.1           |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,661) | 1:7:A:ALA:H  | 1:6:A:THR:HA    | 30       | 0.1           |
| (3,661) | 1:7:A:ALA:H  | 1:6:A:THR:HA    | 32       | 0.1           |
| (3,609) | 1:43:A:TYR:H | 1:42:A:TRP:HB2  | 7        | 0.1           |
| (3,609) | 1:43:A:TYR:H | 1:42:A:TRP:HB2  | 16       | 0.1           |
| (3,609) | 1:43:A:TYR:H | 1:42:A:TRP:HB2  | 39       | 0.1           |
| (3,609) | 1:43:A:TYR:H | 1:42:A:TRP:HB2  | 40       | 0.1           |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 6        | 0.1           |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 6        | 0.1           |
| (3,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 6        | 0.1           |
| (3,564) | 1:47:A:THR:H | 1:43:A:TYR:HB3  | 10       | 0.1           |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 3        | 0.1           |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 3        | 0.1           |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 3        | 0.1           |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 6        | 0.1           |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 6        | 0.1           |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 6        | 0.1           |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 12       | 0.1           |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 12       | 0.1           |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 12       | 0.1           |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 19       | 0.1           |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 19       | 0.1           |
| (3,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 19       | 0.1           |
| (3,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 37       | 0.1           |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 6        | 0.1           |
| (3,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 39       | 0.1           |
| (3,419) | 1:69:A:HIS:H | 1:54:A:LYS:HA   | 16       | 0.1           |
| (3,419) | 1:69:A:HIS:H | 1:54:A:LYS:HA   | 27       | 0.1           |
| (3,419) | 1:69:A:HIS:H | 1:54:A:LYS:HA   | 29       | 0.1           |
| (3,419) | 1:69:A:HIS:H | 1:54:A:LYS:HA   | 39       | 0.1           |
| (3,410) | 1:96:A:GLU:H | 1:18:A:ASN:HD21 | 1        | 0.1           |
| (3,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 4        | 0.1           |
| (3,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 12       | 0.1           |
| (3,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 31       | 0.1           |
| (3,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 32       | 0.1           |
| (3,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 34       | 0.1           |
| (3,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 38       | 0.1           |
| (3,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD1  | 6        | 0.1           |
| (3,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD2  | 6        | 0.1           |
| (3,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD1  | 15       | 0.1           |
| (3,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD2  | 15       | 0.1           |
| (3,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD1  | 26       | 0.1           |
| (3,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD2  | 26       | 0.1           |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (3,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD1  | 28       | 0.1           |
| (3,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD2  | 28       | 0.1           |
| (3,314) | 1:63:A:CYS:H | 1:64:A:HIS:HD2  | 16       | 0.1           |
| (3,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 8        | 0.1           |
| (3,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 10       | 0.1           |
| (3,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 13       | 0.1           |
| (3,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3  | 3        | 0.1           |
| (3,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3  | 10       | 0.1           |
| (3,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3  | 13       | 0.1           |
| (3,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3  | 15       | 0.1           |
| (3,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3  | 17       | 0.1           |
| (3,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3  | 24       | 0.1           |
| (3,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3  | 25       | 0.1           |
| (3,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3  | 26       | 0.1           |
| (3,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3  | 30       | 0.1           |
| (3,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3  | 34       | 0.1           |
| (3,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3  | 36       | 0.1           |
| (3,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3  | 39       | 0.1           |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG21 | 28       | 0.1           |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG22 | 28       | 0.1           |
| (3,252) | 1:95:A:ALA:H | 1:94:A:THR:HG23 | 28       | 0.1           |
| (3,239) | 1:13:A:THR:H | 1:14:A:LYS:HA   | 1        | 0.1           |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1  | 11       | 0.1           |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2  | 11       | 0.1           |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1  | 13       | 0.1           |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2  | 13       | 0.1           |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1  | 26       | 0.1           |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2  | 26       | 0.1           |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1  | 38       | 0.1           |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2  | 38       | 0.1           |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD1  | 39       | 0.1           |
| (3,230) | 1:13:A:THR:H | 1:12:A:PHE:HD2  | 39       | 0.1           |
| (3,212) | 1:91:A:ALA:H | 1:90:A:GLU:HB2  | 6        | 0.1           |
| (3,203) | 1:90:A:GLU:H | 1:91:A:ALA:H    | 3        | 0.1           |
| (3,203) | 1:90:A:GLU:H | 1:91:A:ALA:H    | 6        | 0.1           |
| (3,203) | 1:90:A:GLU:H | 1:91:A:ALA:H    | 7        | 0.1           |
| (3,203) | 1:90:A:GLU:H | 1:91:A:ALA:H    | 10       | 0.1           |
| (3,203) | 1:90:A:GLU:H | 1:91:A:ALA:H    | 16       | 0.1           |
| (3,203) | 1:90:A:GLU:H | 1:91:A:ALA:H    | 20       | 0.1           |
| (3,201) | 1:90:A:GLU:H | 1:89:A:GLY:HA2  | 14       | 0.1           |
| (3,198) | 1:90:A:GLU:H | 1:90:A:GLU:HB2  | 2        | 0.1           |
| (3,198) | 1:90:A:GLU:H | 1:90:A:GLU:HB2  | 13       | 0.1           |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (3,165)  | 1:10:A:ILE:H   | 1:9:A:PRO:HB2   | 3        | 0.1           |
| (3,165)  | 1:10:A:ILE:H   | 1:9:A:PRO:HB2   | 4        | 0.1           |
| (3,165)  | 1:10:A:ILE:H   | 1:9:A:PRO:HB2   | 5        | 0.1           |
| (3,165)  | 1:10:A:ILE:H   | 1:9:A:PRO:HB2   | 12       | 0.1           |
| (3,165)  | 1:10:A:ILE:H   | 1:9:A:PRO:HB2   | 19       | 0.1           |
| (3,141)  | 1:101:A:LEU:H  | 1:100:A:GLU:H   | 22       | 0.1           |
| (3,113)  | 1:63:A:CYS:H   | 1:60:A:ASP:H    | 10       | 0.1           |
| (3,57)   | 1:42:A:TRP:H   | 1:42:A:TRP:HB3  | 9        | 0.1           |
| (3,57)   | 1:42:A:TRP:H   | 1:42:A:TRP:HB3  | 11       | 0.1           |
| (3,57)   | 1:42:A:TRP:H   | 1:42:A:TRP:HB3  | 13       | 0.1           |
| (3,57)   | 1:42:A:TRP:H   | 1:42:A:TRP:HB3  | 15       | 0.1           |
| (3,57)   | 1:42:A:TRP:H   | 1:42:A:TRP:HB3  | 26       | 0.1           |
| (3,57)   | 1:42:A:TRP:H   | 1:42:A:TRP:HB3  | 28       | 0.1           |
| (3,57)   | 1:42:A:TRP:H   | 1:42:A:TRP:HB3  | 32       | 0.1           |
| (3,57)   | 1:42:A:TRP:H   | 1:42:A:TRP:HB3  | 35       | 0.1           |
| (3,24)   | 1:89:A:GLY:H   | 1:9:A:PRO:HB3   | 6        | 0.1           |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 1        | 0.1           |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 1        | 0.1           |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 3        | 0.1           |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 3        | 0.1           |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD1  | 22       | 0.1           |
| (1,3209) | 1:57:A:PHE:HZ  | 1:55:A:TYR:HD2  | 22       | 0.1           |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG21 | 1        | 0.1           |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG22 | 1        | 0.1           |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG23 | 1        | 0.1           |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG21 | 32       | 0.1           |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG22 | 32       | 0.1           |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG23 | 32       | 0.1           |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG21 | 34       | 0.1           |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG22 | 34       | 0.1           |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG23 | 34       | 0.1           |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG21 | 35       | 0.1           |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG22 | 35       | 0.1           |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG23 | 35       | 0.1           |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG21 | 36       | 0.1           |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG22 | 36       | 0.1           |
| (1,3194) | 1:29:A:PHE:HZ  | 1:19:A:ILE:HG23 | 36       | 0.1           |
| (1,3185) | 1:43:A:TYR:HD1 | 1:44:A:LYS:H    | 2        | 0.1           |
| (1,3185) | 1:43:A:TYR:HD2 | 1:44:A:LYS:H    | 2        | 0.1           |
| (1,3185) | 1:43:A:TYR:HD1 | 1:44:A:LYS:H    | 6        | 0.1           |
| (1,3185) | 1:43:A:TYR:HD2 | 1:44:A:LYS:H    | 6        | 0.1           |
| (1,3183) | 1:43:A:TYR:HE1 | 1:82:A:ILE:HG13 | 14       | 0.1           |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3183) | 1:43:A:TYR:HE2 | 1:82:A:ILE:HG13 | 14       | 0.1           |
| (1,3183) | 1:43:A:TYR:HE1 | 1:82:A:ILE:HG13 | 17       | 0.1           |
| (1,3183) | 1:43:A:TYR:HE2 | 1:82:A:ILE:HG13 | 17       | 0.1           |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 3        | 0.1           |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 3        | 0.1           |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 3        | 0.1           |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE1  | 37       | 0.1           |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE2  | 37       | 0.1           |
| (1,3176) | 1:42:A:TRP:HE1 | 1:66:A:MET:HE3  | 37       | 0.1           |
| (1,3158) | 1:42:A:TRP:HD1 | 1:41:A:THR:HA   | 10       | 0.1           |
| (1,3137) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3  | 5        | 0.1           |
| (1,3137) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 5        | 0.1           |
| (1,3137) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3  | 13       | 0.1           |
| (1,3137) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 13       | 0.1           |
| (1,3137) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3  | 21       | 0.1           |
| (1,3137) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 21       | 0.1           |
| (1,3137) | 1:65:A:TYR:HD1 | 1:30:A:GLU:HB3  | 31       | 0.1           |
| (1,3137) | 1:65:A:TYR:HD2 | 1:30:A:GLU:HB3  | 31       | 0.1           |
| (1,3134) | 1:65:A:TYR:HE1 | 1:30:A:GLU:HB2  | 40       | 0.1           |
| (1,3134) | 1:65:A:TYR:HE2 | 1:30:A:GLU:HB2  | 40       | 0.1           |
| (1,3133) | 1:65:A:TYR:HE1 | 1:60:A:ASP:HB3  | 6        | 0.1           |
| (1,3133) | 1:65:A:TYR:HE2 | 1:60:A:ASP:HB3  | 6        | 0.1           |
| (1,3133) | 1:65:A:TYR:HE1 | 1:60:A:ASP:HB3  | 12       | 0.1           |
| (1,3133) | 1:65:A:TYR:HE2 | 1:60:A:ASP:HB3  | 12       | 0.1           |
| (1,3131) | 1:65:A:TYR:HE1 | 1:63:A:CYS:HB3  | 18       | 0.1           |
| (1,3131) | 1:65:A:TYR:HE2 | 1:63:A:CYS:HB3  | 18       | 0.1           |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG21 | 5        | 0.1           |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG22 | 5        | 0.1           |
| (1,3118) | 1:55:A:TYR:HD1 | 1:68:A:ILE:HG23 | 5        | 0.1           |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG21 | 5        | 0.1           |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG22 | 5        | 0.1           |
| (1,3118) | 1:55:A:TYR:HD2 | 1:68:A:ILE:HG23 | 5        | 0.1           |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG21 | 12       | 0.1           |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG22 | 12       | 0.1           |
| (1,3116) | 1:55:A:TYR:HE1 | 1:68:A:ILE:HG23 | 12       | 0.1           |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG21 | 12       | 0.1           |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG22 | 12       | 0.1           |
| (1,3116) | 1:55:A:TYR:HE2 | 1:68:A:ILE:HG23 | 12       | 0.1           |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD1  | 4        | 0.1           |
| (1,3100) | 1:79:A:TYR:HE1 | 1:55:A:TYR:HD2  | 4        | 0.1           |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD1  | 4        | 0.1           |
| (1,3100) | 1:79:A:TYR:HE2 | 1:55:A:TYR:HD2  | 4        | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3092) | 1:66:A:MET:HE1  | 1:55:A:TYR:HE1  | 37       | 0.1           |
| (1,3092) | 1:66:A:MET:HE1  | 1:55:A:TYR:HE2  | 37       | 0.1           |
| (1,3092) | 1:66:A:MET:HE2  | 1:55:A:TYR:HE1  | 37       | 0.1           |
| (1,3092) | 1:66:A:MET:HE2  | 1:55:A:TYR:HE2  | 37       | 0.1           |
| (1,3092) | 1:66:A:MET:HE3  | 1:55:A:TYR:HE1  | 37       | 0.1           |
| (1,3092) | 1:66:A:MET:HE3  | 1:55:A:TYR:HE2  | 37       | 0.1           |
| (1,3084) | 1:98:A:LYS:HD3  | 1:20:A:VAL:HG21 | 11       | 0.1           |
| (1,3084) | 1:98:A:LYS:HD3  | 1:20:A:VAL:HG22 | 11       | 0.1           |
| (1,3084) | 1:98:A:LYS:HD3  | 1:20:A:VAL:HG23 | 11       | 0.1           |
| (1,3082) | 1:97:A:LEU:HB3  | 1:29:A:PHE:HE1  | 4        | 0.1           |
| (1,3082) | 1:97:A:LEU:HB3  | 1:29:A:PHE:HE2  | 4        | 0.1           |
| (1,3082) | 1:97:A:LEU:HB3  | 1:29:A:PHE:HE1  | 20       | 0.1           |
| (1,3082) | 1:97:A:LEU:HB3  | 1:29:A:PHE:HE2  | 20       | 0.1           |
| (1,3082) | 1:97:A:LEU:HB3  | 1:29:A:PHE:HE1  | 27       | 0.1           |
| (1,3082) | 1:97:A:LEU:HB3  | 1:29:A:PHE:HE2  | 27       | 0.1           |
| (1,3040) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG21 | 12       | 0.1           |
| (1,3040) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG22 | 12       | 0.1           |
| (1,3040) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG23 | 12       | 0.1           |
| (1,3040) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG21 | 21       | 0.1           |
| (1,3040) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG22 | 21       | 0.1           |
| (1,3040) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG23 | 21       | 0.1           |
| (1,3040) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG21 | 40       | 0.1           |
| (1,3040) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG22 | 40       | 0.1           |
| (1,3040) | 1:55:A:TYR:HA   | 1:68:A:ILE:HG23 | 40       | 0.1           |
| (1,3033) | 1:44:A:LYS:HE2  | 1:79:A:TYR:HE1  | 32       | 0.1           |
| (1,3033) | 1:44:A:LYS:HE2  | 1:79:A:TYR:HE2  | 32       | 0.1           |
| (1,3013) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 7        | 0.1           |
| (1,3013) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 7        | 0.1           |
| (1,3013) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 20       | 0.1           |
| (1,3013) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 20       | 0.1           |
| (1,3013) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD1  | 30       | 0.1           |
| (1,3013) | 1:30:A:GLU:HG2  | 1:65:A:TYR:HD2  | 30       | 0.1           |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG21 | 3        | 0.1           |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG22 | 3        | 0.1           |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG23 | 3        | 0.1           |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG21 | 14       | 0.1           |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG22 | 14       | 0.1           |
| (1,3012) | 1:30:A:GLU:HG3  | 1:28:A:THR:HG23 | 14       | 0.1           |
| (1,3011) | 1:30:A:GLU:HB2  | 1:14:A:LYS:HE2  | 8        | 0.1           |
| (1,3011) | 1:30:A:GLU:HB2  | 1:14:A:LYS:HE2  | 12       | 0.1           |
| (1,3009) | 1:102:A:ARG:HD3 | 1:102:A:ARG:HB2 | 19       | 0.1           |
| (1,2996) | 1:15:A:ARG:HG2  | 1:93:A:SER:HB3  | 2        | 0.1           |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,2974) | 1:65:A:TYR:HA  | 1:42:A:TRP:HZ2  | 2        | 0.1           |
| (1,2974) | 1:65:A:TYR:HA  | 1:42:A:TRP:HZ2  | 5        | 0.1           |
| (1,2974) | 1:65:A:TYR:HA  | 1:42:A:TRP:HZ2  | 27       | 0.1           |
| (1,2974) | 1:65:A:TYR:HA  | 1:42:A:TRP:HZ2  | 36       | 0.1           |
| (1,2949) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HA    | 31       | 0.1           |
| (1,2948) | 1:8:A:GLU:HG2  | 1:8:A:GLU:HB2   | 16       | 0.1           |
| (1,2942) | 1:90:A:GLU:HA  | 1:84:A:ARG:HA   | 14       | 0.1           |
| (1,2940) | 1:44:A:LYS:HB2 | 1:47:A:THR:HG21 | 10       | 0.1           |
| (1,2940) | 1:44:A:LYS:HB2 | 1:47:A:THR:HG22 | 10       | 0.1           |
| (1,2940) | 1:44:A:LYS:HB2 | 1:47:A:THR:HG23 | 10       | 0.1           |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1  | 5        | 0.1           |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2  | 5        | 0.1           |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1  | 13       | 0.1           |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2  | 13       | 0.1           |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1  | 21       | 0.1           |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2  | 21       | 0.1           |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD1  | 31       | 0.1           |
| (1,2937) | 1:30:A:GLU:HB3 | 1:65:A:TYR:HD2  | 31       | 0.1           |
| (1,2931) | 1:26:A:SER:HA  | 1:70:A:ASN:H    | 7        | 0.1           |
| (1,2931) | 1:26:A:SER:HA  | 1:70:A:ASN:H    | 32       | 0.1           |
| (1,2930) | 1:17:A:GLN:HG2 | 1:18:A:ASN:H    | 7        | 0.1           |
| (1,2930) | 1:17:A:GLN:HG2 | 1:18:A:ASN:H    | 22       | 0.1           |
| (1,2910) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HG3  | 16       | 0.1           |
| (1,2910) | 1:98:A:LYS:HE3 | 1:98:A:LYS:HG3  | 37       | 0.1           |
| (1,2841) | 1:84:A:ARG:HG2 | 1:84:A:ARG:HA   | 10       | 0.1           |
| (1,2841) | 1:84:A:ARG:HG2 | 1:84:A:ARG:HA   | 16       | 0.1           |
| (1,2841) | 1:84:A:ARG:HG2 | 1:84:A:ARG:HA   | 21       | 0.1           |
| (1,2841) | 1:84:A:ARG:HG2 | 1:84:A:ARG:HA   | 27       | 0.1           |
| (1,2841) | 1:84:A:ARG:HG2 | 1:84:A:ARG:HA   | 30       | 0.1           |
| (1,2841) | 1:84:A:ARG:HG2 | 1:84:A:ARG:HA   | 39       | 0.1           |
| (1,2802) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2  | 1        | 0.1           |
| (1,2802) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2  | 10       | 0.1           |
| (1,2802) | 1:15:A:ARG:HD3 | 1:15:A:ARG:HB2  | 13       | 0.1           |
| (1,2754) | 1:90:A:GLU:HB3 | 1:91:A:ALA:H    | 18       | 0.1           |
| (1,2754) | 1:90:A:GLU:HB3 | 1:91:A:ALA:H    | 22       | 0.1           |
| (1,2754) | 1:90:A:GLU:HB3 | 1:91:A:ALA:H    | 23       | 0.1           |
| (1,2745) | 1:86:A:GLU:HG2 | 1:86:A:GLU:H    | 35       | 0.1           |
| (1,2745) | 1:86:A:GLU:HG3 | 1:86:A:GLU:H    | 35       | 0.1           |
| (1,2716) | 1:48:A:GLU:HA  | 1:41:A:THR:HG21 | 6        | 0.1           |
| (1,2716) | 1:48:A:GLU:HA  | 1:41:A:THR:HG22 | 6        | 0.1           |
| (1,2716) | 1:48:A:GLU:HA  | 1:41:A:THR:HG23 | 6        | 0.1           |
| (1,2716) | 1:48:A:GLU:HA  | 1:41:A:THR:HG21 | 9        | 0.1           |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,2716) | 1:48:A:GLU:HA  | 1:41:A:THR:HG22 | 9        | 0.1           |
| (1,2716) | 1:48:A:GLU:HA  | 1:41:A:THR:HG23 | 9        | 0.1           |
| (1,2716) | 1:48:A:GLU:HA  | 1:41:A:THR:HG21 | 20       | 0.1           |
| (1,2716) | 1:48:A:GLU:HA  | 1:41:A:THR:HG22 | 20       | 0.1           |
| (1,2716) | 1:48:A:GLU:HA  | 1:41:A:THR:HG23 | 20       | 0.1           |
| (1,2715) | 1:48:A:GLU:HA  | 1:49:A:LEU:HG   | 8        | 0.1           |
| (1,2715) | 1:48:A:GLU:HA  | 1:49:A:LEU:HG   | 27       | 0.1           |
| (1,2699) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA   | 18       | 0.1           |
| (1,2699) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA   | 29       | 0.1           |
| (1,2699) | 1:23:A:GLU:HA  | 1:24:A:HIS:HA   | 37       | 0.1           |
| (1,2686) | 1:8:A:GLU:HB3  | 1:8:A:GLU:HG2   | 31       | 0.1           |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 2        | 0.1           |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 2        | 0.1           |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 2        | 0.1           |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 12       | 0.1           |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 12       | 0.1           |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 12       | 0.1           |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 29       | 0.1           |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 29       | 0.1           |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 29       | 0.1           |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG21 | 34       | 0.1           |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG22 | 34       | 0.1           |
| (1,2663) | 1:25:A:GLN:HB2 | 1:21:A:VAL:HG23 | 34       | 0.1           |
| (1,2649) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 4        | 0.1           |
| (1,2649) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 12       | 0.1           |
| (1,2649) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 31       | 0.1           |
| (1,2649) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 32       | 0.1           |
| (1,2649) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 34       | 0.1           |
| (1,2649) | 1:17:A:GLN:HB2 | 1:18:A:ASN:H    | 38       | 0.1           |
| (1,2646) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3   | 23       | 0.1           |
| (1,2646) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3   | 33       | 0.1           |
| (1,2646) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3   | 34       | 0.1           |
| (1,2646) | 1:9:A:PRO:HB2  | 1:9:A:PRO:HD3   | 40       | 0.1           |
| (1,2609) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 3        | 0.1           |
| (1,2609) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 5        | 0.1           |
| (1,2609) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 12       | 0.1           |
| (1,2608) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 3        | 0.1           |
| (1,2608) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 5        | 0.1           |
| (1,2608) | 1:60:A:ASP:HB3 | 1:60:A:ASP:H    | 12       | 0.1           |
| (1,2550) | 1:92:A:ARG:HA  | 1:83:A:ALA:H    | 15       | 0.1           |
| (1,2544) | 1:70:A:ASN:HA  | 1:24:A:HIS:HA   | 33       | 0.1           |
| (1,2537) | 1:73:A:PRO:HG3 | 1:73:A:PRO:HA   | 28       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2537) | 1:73:A:PRO:HG3  | 1:73:A:PRO:HA   | 32       | 0.1           |
| (1,2431) | 1:82:A:ILE:HB   | 1:41:A:THR:H    | 20       | 0.1           |
| (1,2431) | 1:82:A:ILE:HB   | 1:41:A:THR:H    | 39       | 0.1           |
| (1,2416) | 1:10:A:ILE:HB   | 1:9:A:PRO:HA    | 8        | 0.1           |
| (1,2416) | 1:10:A:ILE:HB   | 1:9:A:PRO:HA    | 14       | 0.1           |
| (1,2416) | 1:10:A:ILE:HB   | 1:9:A:PRO:HA    | 28       | 0.1           |
| (1,2416) | 1:10:A:ILE:HB   | 1:9:A:PRO:HA    | 29       | 0.1           |
| (1,2416) | 1:10:A:ILE:HB   | 1:9:A:PRO:HA    | 31       | 0.1           |
| (1,2403) | 1:66:A:MET:HE1  | 1:42:A:TRP:H    | 21       | 0.1           |
| (1,2403) | 1:66:A:MET:HE2  | 1:42:A:TRP:H    | 21       | 0.1           |
| (1,2403) | 1:66:A:MET:HE3  | 1:42:A:TRP:H    | 21       | 0.1           |
| (1,2402) | 1:66:A:MET:HE1  | 1:29:A:PHE:HZ   | 28       | 0.1           |
| (1,2402) | 1:66:A:MET:HE2  | 1:29:A:PHE:HZ   | 28       | 0.1           |
| (1,2402) | 1:66:A:MET:HE3  | 1:29:A:PHE:HZ   | 28       | 0.1           |
| (1,2402) | 1:66:A:MET:HE1  | 1:29:A:PHE:HZ   | 29       | 0.1           |
| (1,2402) | 1:66:A:MET:HE2  | 1:29:A:PHE:HZ   | 29       | 0.1           |
| (1,2402) | 1:66:A:MET:HE3  | 1:29:A:PHE:HZ   | 29       | 0.1           |
| (1,2331) | 1:26:A:SER:HA   | 1:68:A:ILE:HG21 | 24       | 0.1           |
| (1,2331) | 1:26:A:SER:HA   | 1:68:A:ILE:HG22 | 24       | 0.1           |
| (1,2331) | 1:26:A:SER:HA   | 1:68:A:ILE:HG23 | 24       | 0.1           |
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG21 | 4        | 0.1           |
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG22 | 4        | 0.1           |
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG23 | 4        | 0.1           |
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG21 | 25       | 0.1           |
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG22 | 25       | 0.1           |
| (1,2265) | 1:96:A:GLU:HB3  | 1:78:A:VAL:HG23 | 25       | 0.1           |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD11 | 23       | 0.1           |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD12 | 23       | 0.1           |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD13 | 23       | 0.1           |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD11 | 29       | 0.1           |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD12 | 29       | 0.1           |
| (1,2165) | 1:35:A:PHE:HB3  | 1:10:A:ILE:HD13 | 29       | 0.1           |
| (1,2145) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 4        | 0.1           |
| (1,2145) | 1:94:A:THR:HA   | 1:81:A:VAL:H    | 17       | 0.1           |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE1  | 13       | 0.1           |
| (1,2077) | 1:97:A:LEU:HD11 | 1:29:A:PHE:HE2  | 13       | 0.1           |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE1  | 13       | 0.1           |
| (1,2077) | 1:97:A:LEU:HD12 | 1:29:A:PHE:HE2  | 13       | 0.1           |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE1  | 13       | 0.1           |
| (1,2077) | 1:97:A:LEU:HD13 | 1:29:A:PHE:HE2  | 13       | 0.1           |
| (1,2070) | 1:97:A:LEU:HB2  | 1:19:A:ILE:HB   | 1        | 0.1           |
| (1,2070) | 1:97:A:LEU:HB2  | 1:19:A:ILE:HB   | 10       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD11 | 19       | 0.1           |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD12 | 19       | 0.1           |
| (1,2066) | 1:85:A:LEU:HD11 | 1:10:A:ILE:HD13 | 19       | 0.1           |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD11 | 19       | 0.1           |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD12 | 19       | 0.1           |
| (1,2066) | 1:85:A:LEU:HD12 | 1:10:A:ILE:HD13 | 19       | 0.1           |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD11 | 19       | 0.1           |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD12 | 19       | 0.1           |
| (1,2066) | 1:85:A:LEU:HD13 | 1:10:A:ILE:HD13 | 19       | 0.1           |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE1  | 4        | 0.1           |
| (1,2041) | 1:66:A:MET:HE1  | 1:29:A:PHE:HE2  | 4        | 0.1           |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE1  | 4        | 0.1           |
| (1,2041) | 1:66:A:MET:HE2  | 1:29:A:PHE:HE2  | 4        | 0.1           |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE1  | 4        | 0.1           |
| (1,2041) | 1:66:A:MET:HE3  | 1:29:A:PHE:HE2  | 4        | 0.1           |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3  | 19       | 0.1           |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3  | 19       | 0.1           |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3  | 19       | 0.1           |
| (1,2021) | 1:50:A:THR:HG21 | 1:48:A:GLU:HG3  | 26       | 0.1           |
| (1,2021) | 1:50:A:THR:HG22 | 1:48:A:GLU:HG3  | 26       | 0.1           |
| (1,2021) | 1:50:A:THR:HG23 | 1:48:A:GLU:HG3  | 26       | 0.1           |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 8        | 0.1           |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 10       | 0.1           |
| (1,2007) | 1:30:A:GLU:HB3  | 1:31:A:CYS:H    | 13       | 0.1           |
| (1,2004) | 1:28:A:THR:HG21 | 1:65:A:TYR:HB2  | 26       | 0.1           |
| (1,2004) | 1:28:A:THR:HG22 | 1:65:A:TYR:HB2  | 26       | 0.1           |
| (1,2004) | 1:28:A:THR:HG23 | 1:65:A:TYR:HB2  | 26       | 0.1           |
| (1,1990) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 17       | 0.1           |
| (1,1990) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 17       | 0.1           |
| (1,1990) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 17       | 0.1           |
| (1,1990) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HB3 | 22       | 0.1           |
| (1,1990) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HB3 | 22       | 0.1           |
| (1,1990) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HB3 | 22       | 0.1           |
| (1,1978) | 1:16:A:ILE:HG21 | 1:30:A:GLU:H    | 11       | 0.1           |
| (1,1978) | 1:16:A:ILE:HG22 | 1:30:A:GLU:H    | 11       | 0.1           |
| (1,1978) | 1:16:A:ILE:HG23 | 1:30:A:GLU:H    | 11       | 0.1           |
| (1,1962) | 1:98:A:LYS:HG2  | 1:20:A:VAL:HA   | 21       | 0.1           |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H    | 3        | 0.1           |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H    | 3        | 0.1           |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H    | 3        | 0.1           |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H    | 6        | 0.1           |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H    | 6        | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H    | 6        | 0.1           |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H    | 16       | 0.1           |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H    | 16       | 0.1           |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H    | 16       | 0.1           |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H    | 31       | 0.1           |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H    | 31       | 0.1           |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H    | 31       | 0.1           |
| (1,1919) | 1:50:A:THR:HG21 | 1:51:A:GLU:H    | 40       | 0.1           |
| (1,1919) | 1:50:A:THR:HG22 | 1:51:A:GLU:H    | 40       | 0.1           |
| (1,1919) | 1:50:A:THR:HG23 | 1:51:A:GLU:H    | 40       | 0.1           |
| (1,1909) | 1:10:A:ILE:HD11 | 1:85:A:LEU:HD11 | 14       | 0.1           |
| (1,1909) | 1:10:A:ILE:HD11 | 1:85:A:LEU:HD12 | 14       | 0.1           |
| (1,1909) | 1:10:A:ILE:HD11 | 1:85:A:LEU:HD13 | 14       | 0.1           |
| (1,1909) | 1:10:A:ILE:HD12 | 1:85:A:LEU:HD11 | 14       | 0.1           |
| (1,1909) | 1:10:A:ILE:HD12 | 1:85:A:LEU:HD12 | 14       | 0.1           |
| (1,1909) | 1:10:A:ILE:HD12 | 1:85:A:LEU:HD13 | 14       | 0.1           |
| (1,1909) | 1:10:A:ILE:HD13 | 1:85:A:LEU:HD11 | 14       | 0.1           |
| (1,1909) | 1:10:A:ILE:HD13 | 1:85:A:LEU:HD12 | 14       | 0.1           |
| (1,1909) | 1:10:A:ILE:HD13 | 1:85:A:LEU:HD13 | 14       | 0.1           |
| (1,1903) | 1:66:A:MET:HE1  | 1:79:A:TYR:HA   | 19       | 0.1           |
| (1,1903) | 1:66:A:MET:HE2  | 1:79:A:TYR:HA   | 19       | 0.1           |
| (1,1903) | 1:66:A:MET:HE3  | 1:79:A:TYR:HA   | 19       | 0.1           |
| (1,1903) | 1:66:A:MET:HE1  | 1:79:A:TYR:HA   | 28       | 0.1           |
| (1,1903) | 1:66:A:MET:HE2  | 1:79:A:TYR:HA   | 28       | 0.1           |
| (1,1903) | 1:66:A:MET:HE3  | 1:79:A:TYR:HA   | 28       | 0.1           |
| (1,1896) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3  | 3        | 0.1           |
| (1,1896) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3  | 3        | 0.1           |
| (1,1896) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3  | 3        | 0.1           |
| (1,1896) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3  | 9        | 0.1           |
| (1,1896) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3  | 9        | 0.1           |
| (1,1896) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3  | 9        | 0.1           |
| (1,1896) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3  | 17       | 0.1           |
| (1,1896) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3  | 17       | 0.1           |
| (1,1896) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3  | 17       | 0.1           |
| (1,1896) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3  | 32       | 0.1           |
| (1,1896) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3  | 32       | 0.1           |
| (1,1896) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3  | 32       | 0.1           |
| (1,1896) | 1:47:A:THR:HG21 | 1:44:A:LYS:HB3  | 35       | 0.1           |
| (1,1896) | 1:47:A:THR:HG22 | 1:44:A:LYS:HB3  | 35       | 0.1           |
| (1,1896) | 1:47:A:THR:HG23 | 1:44:A:LYS:HB3  | 35       | 0.1           |
| (1,1863) | 1:7:A:ALA:HB1   | 1:8:A:GLU:H     | 31       | 0.1           |
| (1,1863) | 1:7:A:ALA:HB2   | 1:8:A:GLU:H     | 31       | 0.1           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1863) | 1:7:A:ALA:HB3    | 1:8:A:GLU:H     | 31       | 0.1           |
| (1,1861) | 1:7:A:ALA:HB1    | 1:88:A:ARG:HA   | 23       | 0.1           |
| (1,1861) | 1:7:A:ALA:HB2    | 1:88:A:ARG:HA   | 23       | 0.1           |
| (1,1861) | 1:7:A:ALA:HB3    | 1:88:A:ARG:HA   | 23       | 0.1           |
| (1,1853) | 1:27:A:ALA:HB1   | 1:28:A:THR:H    | 5        | 0.1           |
| (1,1853) | 1:27:A:ALA:HB2   | 1:28:A:THR:H    | 5        | 0.1           |
| (1,1853) | 1:27:A:ALA:HB3   | 1:28:A:THR:H    | 5        | 0.1           |
| (1,1847) | 1:27:A:ALA:HB1   | 1:19:A:ILE:HG21 | 14       | 0.1           |
| (1,1847) | 1:27:A:ALA:HB1   | 1:19:A:ILE:HG22 | 14       | 0.1           |
| (1,1847) | 1:27:A:ALA:HB1   | 1:19:A:ILE:HG23 | 14       | 0.1           |
| (1,1847) | 1:27:A:ALA:HB2   | 1:19:A:ILE:HG21 | 14       | 0.1           |
| (1,1847) | 1:27:A:ALA:HB2   | 1:19:A:ILE:HG22 | 14       | 0.1           |
| (1,1847) | 1:27:A:ALA:HB2   | 1:19:A:ILE:HG23 | 14       | 0.1           |
| (1,1847) | 1:27:A:ALA:HB3   | 1:19:A:ILE:HG21 | 14       | 0.1           |
| (1,1847) | 1:27:A:ALA:HB3   | 1:19:A:ILE:HG22 | 14       | 0.1           |
| (1,1847) | 1:27:A:ALA:HB3   | 1:19:A:ILE:HG23 | 14       | 0.1           |
| (1,1725) | 1:38:A:ALA:HB1   | 1:83:A:ALA:HA   | 4        | 0.1           |
| (1,1725) | 1:38:A:ALA:HB2   | 1:83:A:ALA:HA   | 4        | 0.1           |
| (1,1725) | 1:38:A:ALA:HB3   | 1:83:A:ALA:HA   | 4        | 0.1           |
| (1,1696) | 1:101:A:LEU:HD21 | 1:101:A:LEU:HB3 | 15       | 0.1           |
| (1,1696) | 1:101:A:LEU:HD22 | 1:101:A:LEU:HB3 | 15       | 0.1           |
| (1,1696) | 1:101:A:LEU:HD23 | 1:101:A:LEU:HB3 | 15       | 0.1           |
| (1,1696) | 1:101:A:LEU:HD21 | 1:101:A:LEU:HB3 | 26       | 0.1           |
| (1,1696) | 1:101:A:LEU:HD22 | 1:101:A:LEU:HB3 | 26       | 0.1           |
| (1,1696) | 1:101:A:LEU:HD23 | 1:101:A:LEU:HB3 | 26       | 0.1           |
| (1,1685) | 1:97:A:LEU:HD11  | 1:71:A:VAL:HG21 | 4        | 0.1           |
| (1,1685) | 1:97:A:LEU:HD11  | 1:71:A:VAL:HG22 | 4        | 0.1           |
| (1,1685) | 1:97:A:LEU:HD11  | 1:71:A:VAL:HG23 | 4        | 0.1           |
| (1,1685) | 1:97:A:LEU:HD12  | 1:71:A:VAL:HG21 | 4        | 0.1           |
| (1,1685) | 1:97:A:LEU:HD12  | 1:71:A:VAL:HG22 | 4        | 0.1           |
| (1,1685) | 1:97:A:LEU:HD12  | 1:71:A:VAL:HG23 | 4        | 0.1           |
| (1,1685) | 1:97:A:LEU:HD13  | 1:71:A:VAL:HG21 | 4        | 0.1           |
| (1,1685) | 1:97:A:LEU:HD13  | 1:71:A:VAL:HG22 | 4        | 0.1           |
| (1,1685) | 1:97:A:LEU:HD13  | 1:71:A:VAL:HG23 | 4        | 0.1           |
| (1,1685) | 1:97:A:LEU:HD11  | 1:71:A:VAL:HG21 | 16       | 0.1           |
| (1,1685) | 1:97:A:LEU:HD11  | 1:71:A:VAL:HG22 | 16       | 0.1           |
| (1,1685) | 1:97:A:LEU:HD11  | 1:71:A:VAL:HG23 | 16       | 0.1           |
| (1,1685) | 1:97:A:LEU:HD12  | 1:71:A:VAL:HG21 | 16       | 0.1           |
| (1,1685) | 1:97:A:LEU:HD12  | 1:71:A:VAL:HG22 | 16       | 0.1           |
| (1,1685) | 1:97:A:LEU:HD12  | 1:71:A:VAL:HG23 | 16       | 0.1           |
| (1,1685) | 1:97:A:LEU:HD13  | 1:71:A:VAL:HG21 | 16       | 0.1           |
| (1,1685) | 1:97:A:LEU:HD13  | 1:71:A:VAL:HG22 | 16       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1685) | 1:97:A:LEU:HD13 | 1:71:A:VAL:HG23 | 16       | 0.1           |
| (1,1679) | 1:85:A:LEU:HD11 | 1:35:A:PHE:HD1  | 14       | 0.1           |
| (1,1679) | 1:85:A:LEU:HD11 | 1:35:A:PHE:HD2  | 14       | 0.1           |
| (1,1679) | 1:85:A:LEU:HD12 | 1:35:A:PHE:HD1  | 14       | 0.1           |
| (1,1679) | 1:85:A:LEU:HD12 | 1:35:A:PHE:HD2  | 14       | 0.1           |
| (1,1679) | 1:85:A:LEU:HD13 | 1:35:A:PHE:HD1  | 14       | 0.1           |
| (1,1679) | 1:85:A:LEU:HD13 | 1:35:A:PHE:HD2  | 14       | 0.1           |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 34       | 0.1           |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 34       | 0.1           |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 34       | 0.1           |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 38       | 0.1           |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 38       | 0.1           |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 38       | 0.1           |
| (1,1678) | 1:85:A:LEU:HD11 | 1:85:A:LEU:HA   | 40       | 0.1           |
| (1,1678) | 1:85:A:LEU:HD12 | 1:85:A:LEU:HA   | 40       | 0.1           |
| (1,1678) | 1:85:A:LEU:HD13 | 1:85:A:LEU:HA   | 40       | 0.1           |
| (1,1650) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 2        | 0.1           |
| (1,1650) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 2        | 0.1           |
| (1,1650) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 2        | 0.1           |
| (1,1650) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 2        | 0.1           |
| (1,1650) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 2        | 0.1           |
| (1,1650) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 2        | 0.1           |
| (1,1650) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 2        | 0.1           |
| (1,1650) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 2        | 0.1           |
| (1,1650) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 2        | 0.1           |
| (1,1650) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG21 | 38       | 0.1           |
| (1,1650) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG22 | 38       | 0.1           |
| (1,1650) | 1:81:A:VAL:HG21 | 1:16:A:ILE:HG23 | 38       | 0.1           |
| (1,1650) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG21 | 38       | 0.1           |
| (1,1650) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG22 | 38       | 0.1           |
| (1,1650) | 1:81:A:VAL:HG22 | 1:16:A:ILE:HG23 | 38       | 0.1           |
| (1,1650) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG21 | 38       | 0.1           |
| (1,1650) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG22 | 38       | 0.1           |
| (1,1650) | 1:81:A:VAL:HG23 | 1:16:A:ILE:HG23 | 38       | 0.1           |
| (1,1622) | 1:82:A:ILE:HD11 | 1:83:A:ALA:H    | 11       | 0.1           |
| (1,1622) | 1:82:A:ILE:HD12 | 1:83:A:ALA:H    | 11       | 0.1           |
| (1,1622) | 1:82:A:ILE:HD13 | 1:83:A:ALA:H    | 11       | 0.1           |
| (1,1622) | 1:82:A:ILE:HD11 | 1:83:A:ALA:H    | 28       | 0.1           |
| (1,1622) | 1:82:A:ILE:HD12 | 1:83:A:ALA:H    | 28       | 0.1           |
| (1,1622) | 1:82:A:ILE:HD13 | 1:83:A:ALA:H    | 28       | 0.1           |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD1  | 5        | 0.1           |
| (1,1601) | 1:68:A:ILE:HG21 | 1:55:A:TYR:HD2  | 5        | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD1  | 5        | 0.1           |
| (1,1601) | 1:68:A:ILE:HG22 | 1:55:A:TYR:HD2  | 5        | 0.1           |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD1  | 5        | 0.1           |
| (1,1601) | 1:68:A:ILE:HG23 | 1:55:A:TYR:HD2  | 5        | 0.1           |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE1  | 10       | 0.1           |
| (1,1600) | 1:68:A:ILE:HG21 | 1:79:A:TYR:HE2  | 10       | 0.1           |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE1  | 10       | 0.1           |
| (1,1600) | 1:68:A:ILE:HG22 | 1:79:A:TYR:HE2  | 10       | 0.1           |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE1  | 10       | 0.1           |
| (1,1600) | 1:68:A:ILE:HG23 | 1:79:A:TYR:HE2  | 10       | 0.1           |
| (1,1550) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA    | 19       | 0.1           |
| (1,1550) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA    | 19       | 0.1           |
| (1,1550) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA    | 19       | 0.1           |
| (1,1550) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA    | 30       | 0.1           |
| (1,1550) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA    | 30       | 0.1           |
| (1,1550) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA    | 30       | 0.1           |
| (1,1550) | 1:10:A:ILE:HG21 | 1:9:A:PRO:HA    | 35       | 0.1           |
| (1,1550) | 1:10:A:ILE:HG22 | 1:9:A:PRO:HA    | 35       | 0.1           |
| (1,1550) | 1:10:A:ILE:HG23 | 1:9:A:PRO:HA    | 35       | 0.1           |
| (1,1513) | 1:66:A:MET:HE1  | 1:29:A:PHE:H    | 27       | 0.1           |
| (1,1513) | 1:66:A:MET:HE2  | 1:29:A:PHE:H    | 27       | 0.1           |
| (1,1513) | 1:66:A:MET:HE3  | 1:29:A:PHE:H    | 27       | 0.1           |
| (1,1513) | 1:66:A:MET:HE1  | 1:29:A:PHE:H    | 31       | 0.1           |
| (1,1513) | 1:66:A:MET:HE2  | 1:29:A:PHE:H    | 31       | 0.1           |
| (1,1513) | 1:66:A:MET:HE3  | 1:29:A:PHE:H    | 31       | 0.1           |
| (1,1510) | 1:66:A:MET:HE1  | 1:42:A:TRP:HE1  | 3        | 0.1           |
| (1,1510) | 1:66:A:MET:HE2  | 1:42:A:TRP:HE1  | 3        | 0.1           |
| (1,1510) | 1:66:A:MET:HE3  | 1:42:A:TRP:HE1  | 3        | 0.1           |
| (1,1510) | 1:66:A:MET:HE1  | 1:42:A:TRP:HE1  | 37       | 0.1           |
| (1,1510) | 1:66:A:MET:HE2  | 1:42:A:TRP:HE1  | 37       | 0.1           |
| (1,1510) | 1:66:A:MET:HE3  | 1:42:A:TRP:HE1  | 37       | 0.1           |
| (1,1508) | 1:66:A:MET:HE1  | 1:42:A:TRP:HZ3  | 2        | 0.1           |
| (1,1508) | 1:66:A:MET:HE2  | 1:42:A:TRP:HZ3  | 2        | 0.1           |
| (1,1508) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3  | 2        | 0.1           |
| (1,1508) | 1:66:A:MET:HE1  | 1:42:A:TRP:HZ3  | 24       | 0.1           |
| (1,1508) | 1:66:A:MET:HE2  | 1:42:A:TRP:HZ3  | 24       | 0.1           |
| (1,1508) | 1:66:A:MET:HE3  | 1:42:A:TRP:HZ3  | 24       | 0.1           |
| (1,1507) | 1:66:A:MET:HE1  | 1:42:A:TRP:HB2  | 13       | 0.1           |
| (1,1507) | 1:66:A:MET:HE2  | 1:42:A:TRP:HB2  | 13       | 0.1           |
| (1,1507) | 1:66:A:MET:HE3  | 1:42:A:TRP:HB2  | 13       | 0.1           |
| (1,1502) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD11 | 14       | 0.1           |
| (1,1502) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD12 | 14       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1502) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD13 | 14       | 0.1           |
| (1,1502) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD11 | 14       | 0.1           |
| (1,1502) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD12 | 14       | 0.1           |
| (1,1502) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD13 | 14       | 0.1           |
| (1,1502) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD11 | 14       | 0.1           |
| (1,1502) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD12 | 14       | 0.1           |
| (1,1502) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD13 | 14       | 0.1           |
| (1,1502) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD11 | 26       | 0.1           |
| (1,1502) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD12 | 26       | 0.1           |
| (1,1502) | 1:66:A:MET:HE1  | 1:49:A:LEU:HD13 | 26       | 0.1           |
| (1,1502) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD11 | 26       | 0.1           |
| (1,1502) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD12 | 26       | 0.1           |
| (1,1502) | 1:66:A:MET:HE2  | 1:49:A:LEU:HD13 | 26       | 0.1           |
| (1,1502) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD11 | 26       | 0.1           |
| (1,1502) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD12 | 26       | 0.1           |
| (1,1502) | 1:66:A:MET:HE3  | 1:49:A:LEU:HD13 | 26       | 0.1           |
| (1,1494) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 5        | 0.1           |
| (1,1494) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 5        | 0.1           |
| (1,1494) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 5        | 0.1           |
| (1,1494) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 25       | 0.1           |
| (1,1494) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 25       | 0.1           |
| (1,1494) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 25       | 0.1           |
| (1,1494) | 1:81:A:VAL:HG11 | 1:12:A:PHE:HZ   | 29       | 0.1           |
| (1,1494) | 1:81:A:VAL:HG12 | 1:12:A:PHE:HZ   | 29       | 0.1           |
| (1,1494) | 1:81:A:VAL:HG13 | 1:12:A:PHE:HZ   | 29       | 0.1           |
| (1,1484) | 1:81:A:VAL:HB   | 1:42:A:TRP:HE1  | 4        | 0.1           |
| (1,1484) | 1:81:A:VAL:HB   | 1:42:A:TRP:HE1  | 7        | 0.1           |
| (1,1484) | 1:81:A:VAL:HB   | 1:42:A:TRP:HE1  | 31       | 0.1           |
| (1,1473) | 1:78:A:VAL:HG11 | 1:94:A:THR:HB   | 28       | 0.1           |
| (1,1473) | 1:78:A:VAL:HG12 | 1:94:A:THR:HB   | 28       | 0.1           |
| (1,1473) | 1:78:A:VAL:HG13 | 1:94:A:THR:HB   | 28       | 0.1           |
| (1,1408) | 1:20:A:VAL:HG11 | 1:100:A:GLU:HA  | 33       | 0.1           |
| (1,1408) | 1:20:A:VAL:HG12 | 1:100:A:GLU:HA  | 33       | 0.1           |
| (1,1408) | 1:20:A:VAL:HG13 | 1:100:A:GLU:HA  | 33       | 0.1           |
| (1,1384) | 1:91:A:ALA:HB1  | 1:83:A:ALA:HB1  | 7        | 0.1           |
| (1,1384) | 1:91:A:ALA:HB1  | 1:83:A:ALA:HB2  | 7        | 0.1           |
| (1,1384) | 1:91:A:ALA:HB1  | 1:83:A:ALA:HB3  | 7        | 0.1           |
| (1,1384) | 1:91:A:ALA:HB2  | 1:83:A:ALA:HB1  | 7        | 0.1           |
| (1,1384) | 1:91:A:ALA:HB2  | 1:83:A:ALA:HB2  | 7        | 0.1           |
| (1,1384) | 1:91:A:ALA:HB2  | 1:83:A:ALA:HB3  | 7        | 0.1           |
| (1,1384) | 1:91:A:ALA:HB3  | 1:83:A:ALA:HB1  | 7        | 0.1           |
| (1,1384) | 1:91:A:ALA:HB3  | 1:83:A:ALA:HB2  | 7        | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1384) | 1:91:A:ALA:HB3  | 1:83:A:ALA:HB3  | 7        | 0.1           |
| (1,1379) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB1  | 7        | 0.1           |
| (1,1379) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB2  | 7        | 0.1           |
| (1,1379) | 1:83:A:ALA:HB1  | 1:91:A:ALA:HB3  | 7        | 0.1           |
| (1,1379) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB1  | 7        | 0.1           |
| (1,1379) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB2  | 7        | 0.1           |
| (1,1379) | 1:83:A:ALA:HB2  | 1:91:A:ALA:HB3  | 7        | 0.1           |
| (1,1379) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB1  | 7        | 0.1           |
| (1,1379) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB2  | 7        | 0.1           |
| (1,1379) | 1:83:A:ALA:HB3  | 1:91:A:ALA:HB3  | 7        | 0.1           |
| (1,1368) | 1:16:A:ILE:HB   | 1:29:A:PHE:HB3  | 28       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 1        | 0.1           |
| (1,1357) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 1        | 0.1           |
| (1,1357) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 1        | 0.1           |
| (1,1357) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 3        | 0.1           |
| (1,1357) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 3        | 0.1           |
| (1,1357) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 3        | 0.1           |
| (1,1357) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 4        | 0.1           |
| (1,1357) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 4        | 0.1           |
| (1,1357) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 4        | 0.1           |
| (1,1357) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 6        | 0.1           |
| (1,1357) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 6        | 0.1           |
| (1,1357) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 6        | 0.1           |
| (1,1357) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 11       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 11       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 11       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 12       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 12       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 12       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 13       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 13       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 13       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 14       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 14       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 14       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 20       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 20       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 20       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 23       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 23       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 23       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 25       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1357) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 25       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 25       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 30       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 30       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 30       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 31       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 31       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 31       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 34       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 34       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 34       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 35       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 35       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 35       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 36       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 36       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 36       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG21 | 1:16:A:ILE:HG13 | 40       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG22 | 1:16:A:ILE:HG13 | 40       | 0.1           |
| (1,1357) | 1:16:A:ILE:HG23 | 1:16:A:ILE:HG13 | 40       | 0.1           |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H    | 15       | 0.1           |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H    | 15       | 0.1           |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H    | 15       | 0.1           |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H    | 17       | 0.1           |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H    | 17       | 0.1           |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H    | 17       | 0.1           |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H    | 18       | 0.1           |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H    | 18       | 0.1           |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H    | 18       | 0.1           |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H    | 21       | 0.1           |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H    | 21       | 0.1           |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H    | 21       | 0.1           |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H    | 26       | 0.1           |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H    | 26       | 0.1           |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H    | 26       | 0.1           |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H    | 34       | 0.1           |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H    | 34       | 0.1           |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H    | 34       | 0.1           |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H    | 38       | 0.1           |
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H    | 38       | 0.1           |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H    | 38       | 0.1           |
| (1,1349) | 1:16:A:ILE:HD11 | 1:17:A:GLN:H    | 40       | 0.1           |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1349) | 1:16:A:ILE:HD12 | 1:17:A:GLN:H   | 40       | 0.1           |
| (1,1349) | 1:16:A:ILE:HD13 | 1:17:A:GLN:H   | 40       | 0.1           |
| (1,1348) | 1:16:A:ILE:HD11 | 1:95:A:ALA:H   | 5        | 0.1           |
| (1,1348) | 1:16:A:ILE:HD12 | 1:95:A:ALA:H   | 5        | 0.1           |
| (1,1348) | 1:16:A:ILE:HD13 | 1:95:A:ALA:H   | 5        | 0.1           |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H   | 3        | 0.1           |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H   | 10       | 0.1           |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H   | 27       | 0.1           |
| (1,1295) | 1:40:A:VAL:HB   | 1:41:A:THR:H   | 39       | 0.1           |
| (1,1266) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 28       | 0.1           |
| (1,1266) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 28       | 0.1           |
| (1,1266) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 28       | 0.1           |
| (1,1265) | 1:94:A:THR:HG21 | 1:95:A:ALA:H   | 28       | 0.1           |
| (1,1265) | 1:94:A:THR:HG22 | 1:95:A:ALA:H   | 28       | 0.1           |
| (1,1265) | 1:94:A:THR:HG23 | 1:95:A:ALA:H   | 28       | 0.1           |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA  | 4        | 0.1           |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA  | 4        | 0.1           |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA  | 4        | 0.1           |
| (1,1264) | 1:94:A:THR:HG21 | 1:93:A:SER:HA  | 9        | 0.1           |
| (1,1264) | 1:94:A:THR:HG22 | 1:93:A:SER:HA  | 9        | 0.1           |
| (1,1264) | 1:94:A:THR:HG23 | 1:93:A:SER:HA  | 9        | 0.1           |
| (1,1261) | 1:67:A:THR:HG21 | 1:56:A:ASN:H   | 13       | 0.1           |
| (1,1261) | 1:67:A:THR:HG22 | 1:56:A:ASN:H   | 13       | 0.1           |
| (1,1261) | 1:67:A:THR:HG23 | 1:56:A:ASN:H   | 13       | 0.1           |
| (1,1261) | 1:67:A:THR:HG21 | 1:56:A:ASN:H   | 31       | 0.1           |
| (1,1261) | 1:67:A:THR:HG22 | 1:56:A:ASN:H   | 31       | 0.1           |
| (1,1261) | 1:67:A:THR:HG23 | 1:56:A:ASN:H   | 31       | 0.1           |
| (1,1261) | 1:67:A:THR:HG21 | 1:56:A:ASN:H   | 35       | 0.1           |
| (1,1261) | 1:67:A:THR:HG22 | 1:56:A:ASN:H   | 35       | 0.1           |
| (1,1261) | 1:67:A:THR:HG23 | 1:56:A:ASN:H   | 35       | 0.1           |
| (1,1239) | 1:13:A:THR:HG21 | 1:34:A:SER:H   | 8        | 0.1           |
| (1,1239) | 1:13:A:THR:HG22 | 1:34:A:SER:H   | 8        | 0.1           |
| (1,1239) | 1:13:A:THR:HG23 | 1:34:A:SER:H   | 8        | 0.1           |
| (1,1239) | 1:13:A:THR:HG21 | 1:34:A:SER:H   | 11       | 0.1           |
| (1,1239) | 1:13:A:THR:HG22 | 1:34:A:SER:H   | 11       | 0.1           |
| (1,1239) | 1:13:A:THR:HG23 | 1:34:A:SER:H   | 11       | 0.1           |
| (1,1239) | 1:13:A:THR:HG21 | 1:34:A:SER:H   | 35       | 0.1           |
| (1,1239) | 1:13:A:THR:HG22 | 1:34:A:SER:H   | 35       | 0.1           |
| (1,1239) | 1:13:A:THR:HG23 | 1:34:A:SER:H   | 35       | 0.1           |
| (1,1236) | 1:13:A:THR:HG21 | 1:34:A:SER:HB3 | 33       | 0.1           |
| (1,1236) | 1:13:A:THR:HG22 | 1:34:A:SER:HB3 | 33       | 0.1           |
| (1,1236) | 1:13:A:THR:HG23 | 1:34:A:SER:HB3 | 33       | 0.1           |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1226) | 1:101:A:LEU:H | 1:22:A:SER:HA   | 12       | 0.1           |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD21 | 12       | 0.1           |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD22 | 12       | 0.1           |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD23 | 12       | 0.1           |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD21 | 14       | 0.1           |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD22 | 14       | 0.1           |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD23 | 14       | 0.1           |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD21 | 18       | 0.1           |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD22 | 18       | 0.1           |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD23 | 18       | 0.1           |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD21 | 34       | 0.1           |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD22 | 34       | 0.1           |
| (1,1222) | 1:97:A:LEU:H  | 1:97:A:LEU:HD23 | 34       | 0.1           |
| (1,1217) | 1:69:A:HIS:H  | 1:56:A:ASN:H    | 10       | 0.1           |
| (1,1213) | 1:66:A:MET:H  | 1:28:A:THR:HA   | 15       | 0.1           |
| (1,1213) | 1:66:A:MET:H  | 1:28:A:THR:HA   | 28       | 0.1           |
| (1,1208) | 1:56:A:ASN:H  | 1:66:A:MET:HG2  | 8        | 0.1           |
| (1,1208) | 1:56:A:ASN:H  | 1:66:A:MET:HG2  | 14       | 0.1           |
| (1,1208) | 1:56:A:ASN:H  | 1:66:A:MET:HG2  | 20       | 0.1           |
| (1,1204) | 1:42:A:TRP:H  | 1:57:A:PHE:HE1  | 24       | 0.1           |
| (1,1204) | 1:42:A:TRP:H  | 1:57:A:PHE:HE2  | 24       | 0.1           |
| (1,1202) | 1:41:A:THR:H  | 1:83:A:ALA:HA   | 12       | 0.1           |
| (1,1174) | 1:91:A:ALA:H  | 1:84:A:ARG:HA   | 14       | 0.1           |
| (1,1149) | 1:54:A:LYS:H  | 1:53:A:GLN:HG3  | 14       | 0.1           |
| (1,1149) | 1:54:A:LYS:H  | 1:53:A:GLN:HG3  | 26       | 0.1           |
| (1,1149) | 1:54:A:LYS:H  | 1:53:A:GLN:HG3  | 29       | 0.1           |
| (1,1137) | 1:100:A:GLU:H | 1:101:A:LEU:H   | 22       | 0.1           |
| (1,1130) | 1:40:A:VAL:H  | 1:83:A:ALA:HB1  | 16       | 0.1           |
| (1,1130) | 1:40:A:VAL:H  | 1:83:A:ALA:HB2  | 16       | 0.1           |
| (1,1130) | 1:40:A:VAL:H  | 1:83:A:ALA:HB3  | 16       | 0.1           |
| (1,1056) | 1:33:A:VAL:H  | 1:62:A:ARG:HB2  | 17       | 0.1           |
| (1,1052) | 1:26:A:SER:H  | 1:25:A:GLN:HG2  | 7        | 0.1           |
| (1,1020) | 1:48:A:GLU:H  | 1:48:A:GLU:HG3  | 14       | 0.1           |
| (1,1020) | 1:48:A:GLU:H  | 1:48:A:GLU:HG3  | 30       | 0.1           |
| (1,997)  | 1:79:A:TYR:H  | 1:94:A:THR:HG21 | 6        | 0.1           |
| (1,997)  | 1:79:A:TYR:H  | 1:94:A:THR:HG22 | 6        | 0.1           |
| (1,997)  | 1:79:A:TYR:H  | 1:94:A:THR:HG23 | 6        | 0.1           |
| (1,997)  | 1:79:A:TYR:H  | 1:94:A:THR:HG21 | 18       | 0.1           |
| (1,997)  | 1:79:A:TYR:H  | 1:94:A:THR:HG22 | 18       | 0.1           |
| (1,997)  | 1:79:A:TYR:H  | 1:94:A:THR:HG23 | 18       | 0.1           |
| (1,997)  | 1:79:A:TYR:H  | 1:94:A:THR:HG21 | 20       | 0.1           |
| (1,997)  | 1:79:A:TYR:H  | 1:94:A:THR:HG22 | 20       | 0.1           |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,997) | 1:79:A:TYR:H | 1:94:A:THR:HG23 | 20       | 0.1           |
| (1,987) | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 7        | 0.1           |
| (1,987) | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 13       | 0.1           |
| (1,987) | 1:12:A:PHE:H | 1:11:A:GLN:HB2  | 19       | 0.1           |
| (1,948) | 1:34:A:SER:H | 1:33:A:VAL:HG21 | 20       | 0.1           |
| (1,948) | 1:34:A:SER:H | 1:33:A:VAL:HG22 | 20       | 0.1           |
| (1,948) | 1:34:A:SER:H | 1:33:A:VAL:HG23 | 20       | 0.1           |
| (1,941) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 7        | 0.1           |
| (1,941) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 9        | 0.1           |
| (1,941) | 1:34:A:SER:H | 1:12:A:PHE:HA   | 14       | 0.1           |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 22       | 0.1           |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 22       | 0.1           |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 22       | 0.1           |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 33       | 0.1           |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 33       | 0.1           |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 33       | 0.1           |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 37       | 0.1           |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 37       | 0.1           |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 37       | 0.1           |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG11 | 38       | 0.1           |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG12 | 38       | 0.1           |
| (1,933) | 1:98:A:LYS:H | 1:20:A:VAL:HG13 | 38       | 0.1           |
| (1,915) | 1:37:A:ASP:H | 1:37:A:ASP:HA   | 2        | 0.1           |
| (1,899) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 2        | 0.1           |
| (1,899) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 16       | 0.1           |
| (1,899) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 33       | 0.1           |
| (1,899) | 1:44:A:LYS:H | 1:43:A:TYR:HB2  | 40       | 0.1           |
| (1,889) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 1        | 0.1           |
| (1,889) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 3        | 0.1           |
| (1,889) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 4        | 0.1           |
| (1,889) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 9        | 0.1           |
| (1,889) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 23       | 0.1           |
| (1,889) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 24       | 0.1           |
| (1,889) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 30       | 0.1           |
| (1,889) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 39       | 0.1           |
| (1,889) | 1:80:A:SER:H | 1:79:A:TYR:HB2  | 40       | 0.1           |
| (1,888) | 1:80:A:SER:H | 1:43:A:TYR:HB3  | 33       | 0.1           |
| (1,875) | 1:8:A:GLU:H  | 1:7:A:ALA:HB1   | 31       | 0.1           |
| (1,875) | 1:8:A:GLU:H  | 1:7:A:ALA:HB2   | 31       | 0.1           |
| (1,875) | 1:8:A:GLU:H  | 1:7:A:ALA:HB3   | 31       | 0.1           |
| (1,864) | 1:86:A:GLU:H | 1:86:A:GLU:HG3  | 9        | 0.1           |
| (1,863) | 1:86:A:GLU:H | 1:85:A:LEU:HB3  | 21       | 0.1           |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,863) | 1:86:A:GLU:H | 1:85:A:LEU:HB3  | 36       | 0.1           |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB1  | 39       | 0.1           |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB2  | 39       | 0.1           |
| (1,849) | 1:83:A:ALA:H | 1:91:A:ALA:HB3  | 39       | 0.1           |
| (1,813) | 1:25:A:GLN:H | 1:25:A:GLN:HG3  | 19       | 0.1           |
| (1,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB   | 37       | 0.1           |
| (1,810) | 1:25:A:GLN:H | 1:71:A:VAL:HB   | 38       | 0.1           |
| (1,742) | 1:76:A:GLU:H | 1:77:A:GLY:H    | 6        | 0.1           |
| (1,742) | 1:76:A:GLU:H | 1:77:A:GLY:H    | 9        | 0.1           |
| (1,742) | 1:76:A:GLU:H | 1:77:A:GLY:H    | 13       | 0.1           |
| (1,742) | 1:76:A:GLU:H | 1:77:A:GLY:H    | 19       | 0.1           |
| (1,742) | 1:76:A:GLU:H | 1:77:A:GLY:H    | 37       | 0.1           |
| (1,726) | 1:49:A:LEU:H | 1:48:A:GLU:HG3  | 2        | 0.1           |
| (1,726) | 1:49:A:LEU:H | 1:48:A:GLU:HG3  | 7        | 0.1           |
| (1,726) | 1:49:A:LEU:H | 1:48:A:GLU:HG3  | 11       | 0.1           |
| (1,709) | 1:16:A:ILE:H | 1:31:A:CYS:HB2  | 1        | 0.1           |
| (1,709) | 1:16:A:ILE:H | 1:31:A:CYS:HB2  | 6        | 0.1           |
| (1,666) | 1:72:A:THR:H | 1:72:A:THR:HB   | 8        | 0.1           |
| (1,666) | 1:72:A:THR:H | 1:72:A:THR:HB   | 9        | 0.1           |
| (1,666) | 1:72:A:THR:H | 1:72:A:THR:HB   | 20       | 0.1           |
| (1,666) | 1:72:A:THR:H | 1:72:A:THR:HB   | 30       | 0.1           |
| (1,666) | 1:72:A:THR:H | 1:72:A:THR:HB   | 33       | 0.1           |
| (1,666) | 1:72:A:THR:H | 1:72:A:THR:HB   | 34       | 0.1           |
| (1,666) | 1:72:A:THR:H | 1:72:A:THR:HB   | 35       | 0.1           |
| (1,661) | 1:7:A:ALA:H  | 1:6:A:THR:HA    | 3        | 0.1           |
| (1,661) | 1:7:A:ALA:H  | 1:6:A:THR:HA    | 13       | 0.1           |
| (1,661) | 1:7:A:ALA:H  | 1:6:A:THR:HA    | 29       | 0.1           |
| (1,661) | 1:7:A:ALA:H  | 1:6:A:THR:HA    | 30       | 0.1           |
| (1,661) | 1:7:A:ALA:H  | 1:6:A:THR:HA    | 32       | 0.1           |
| (1,609) | 1:43:A:TYR:H | 1:42:A:TRP:HB2  | 7        | 0.1           |
| (1,609) | 1:43:A:TYR:H | 1:42:A:TRP:HB2  | 16       | 0.1           |
| (1,609) | 1:43:A:TYR:H | 1:42:A:TRP:HB2  | 39       | 0.1           |
| (1,609) | 1:43:A:TYR:H | 1:42:A:TRP:HB2  | 40       | 0.1           |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG21 | 6        | 0.1           |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG22 | 6        | 0.1           |
| (1,567) | 1:47:A:THR:H | 1:47:A:THR:HG23 | 6        | 0.1           |
| (1,564) | 1:47:A:THR:H | 1:43:A:TYR:HB3  | 10       | 0.1           |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 3        | 0.1           |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 3        | 0.1           |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 3        | 0.1           |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 6        | 0.1           |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 6        | 0.1           |

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| Key     | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|---------|--------------|-----------------|----------|---------------|
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 6        | 0.1           |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 12       | 0.1           |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 12       | 0.1           |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 12       | 0.1           |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG11 | 19       | 0.1           |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG12 | 19       | 0.1           |
| (1,551) | 1:71:A:VAL:H | 1:71:A:VAL:HG13 | 19       | 0.1           |
| (1,529) | 1:99:A:GLY:H | 1:76:A:GLU:HB2  | 37       | 0.1           |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 6        | 0.1           |
| (1,512) | 1:67:A:THR:H | 1:66:A:MET:HB2  | 39       | 0.1           |
| (1,419) | 1:69:A:HIS:H | 1:54:A:LYS:HA   | 16       | 0.1           |
| (1,419) | 1:69:A:HIS:H | 1:54:A:LYS:HA   | 27       | 0.1           |
| (1,419) | 1:69:A:HIS:H | 1:54:A:LYS:HA   | 29       | 0.1           |
| (1,419) | 1:69:A:HIS:H | 1:54:A:LYS:HA   | 39       | 0.1           |
| (1,410) | 1:96:A:GLU:H | 1:18:A:ASN:HD21 | 1        | 0.1           |
| (1,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 4        | 0.1           |
| (1,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 12       | 0.1           |
| (1,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 31       | 0.1           |
| (1,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 32       | 0.1           |
| (1,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 34       | 0.1           |
| (1,369) | 1:18:A:ASN:H | 1:17:A:GLN:HB2  | 38       | 0.1           |
| (1,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD1  | 6        | 0.1           |
| (1,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD2  | 6        | 0.1           |
| (1,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD1  | 15       | 0.1           |
| (1,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD2  | 15       | 0.1           |
| (1,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD1  | 26       | 0.1           |
| (1,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD2  | 26       | 0.1           |
| (1,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD1  | 28       | 0.1           |
| (1,339) | 1:14:A:LYS:H | 1:12:A:PHE:HD2  | 28       | 0.1           |
| (1,314) | 1:63:A:CYS:H | 1:64:A:HIS:HD2  | 16       | 0.1           |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 8        | 0.1           |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 10       | 0.1           |
| (1,296) | 1:31:A:CYS:H | 1:30:A:GLU:HB3  | 13       | 0.1           |
| (1,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3  | 3        | 0.1           |
| (1,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3  | 10       | 0.1           |
| (1,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3  | 13       | 0.1           |
| (1,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3  | 15       | 0.1           |
| (1,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3  | 17       | 0.1           |
| (1,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3  | 24       | 0.1           |
| (1,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3  | 25       | 0.1           |
| (1,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3  | 26       | 0.1           |
| (1,281) | 1:29:A:PHE:H | 1:29:A:PHE:HB3  | 30       | 0.1           |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,281) | 1:29:A:PHE:H  | 1:29:A:PHE:HB3  | 34       | 0.1           |
| (1,281) | 1:29:A:PHE:H  | 1:29:A:PHE:HB3  | 36       | 0.1           |
| (1,281) | 1:29:A:PHE:H  | 1:29:A:PHE:HB3  | 39       | 0.1           |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG21 | 28       | 0.1           |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG22 | 28       | 0.1           |
| (1,252) | 1:95:A:ALA:H  | 1:94:A:THR:HG23 | 28       | 0.1           |
| (1,239) | 1:13:A:THR:H  | 1:14:A:LYS:HA   | 1        | 0.1           |
| (1,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD1  | 11       | 0.1           |
| (1,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD2  | 11       | 0.1           |
| (1,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD1  | 13       | 0.1           |
| (1,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD2  | 13       | 0.1           |
| (1,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD1  | 26       | 0.1           |
| (1,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD2  | 26       | 0.1           |
| (1,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD1  | 38       | 0.1           |
| (1,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD2  | 38       | 0.1           |
| (1,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD1  | 39       | 0.1           |
| (1,230) | 1:13:A:THR:H  | 1:12:A:PHE:HD2  | 39       | 0.1           |
| (1,212) | 1:91:A:ALA:H  | 1:90:A:GLU:HB2  | 6        | 0.1           |
| (1,203) | 1:90:A:GLU:H  | 1:91:A:ALA:H    | 3        | 0.1           |
| (1,203) | 1:90:A:GLU:H  | 1:91:A:ALA:H    | 6        | 0.1           |
| (1,203) | 1:90:A:GLU:H  | 1:91:A:ALA:H    | 7        | 0.1           |
| (1,203) | 1:90:A:GLU:H  | 1:91:A:ALA:H    | 10       | 0.1           |
| (1,203) | 1:90:A:GLU:H  | 1:91:A:ALA:H    | 16       | 0.1           |
| (1,203) | 1:90:A:GLU:H  | 1:91:A:ALA:H    | 20       | 0.1           |
| (1,201) | 1:90:A:GLU:H  | 1:89:A:GLY:HA2  | 14       | 0.1           |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG21 | 5        | 0.1           |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG22 | 5        | 0.1           |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG23 | 5        | 0.1           |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG21 | 39       | 0.1           |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG22 | 39       | 0.1           |
| (1,199) | 1:90:A:GLU:H  | 1:10:A:ILE:HG23 | 39       | 0.1           |
| (1,198) | 1:90:A:GLU:H  | 1:90:A:GLU:HB2  | 2        | 0.1           |
| (1,198) | 1:90:A:GLU:H  | 1:90:A:GLU:HB2  | 13       | 0.1           |
| (1,165) | 1:10:A:ILE:H  | 1:9:A:PRO:HB2   | 3        | 0.1           |
| (1,165) | 1:10:A:ILE:H  | 1:9:A:PRO:HB2   | 4        | 0.1           |
| (1,165) | 1:10:A:ILE:H  | 1:9:A:PRO:HB2   | 5        | 0.1           |
| (1,165) | 1:10:A:ILE:H  | 1:9:A:PRO:HB2   | 12       | 0.1           |
| (1,165) | 1:10:A:ILE:H  | 1:9:A:PRO:HB2   | 19       | 0.1           |
| (1,148) | 1:45:A:GLY:H  | 1:46:A:PRO:HD2  | 29       | 0.1           |
| (1,139) | 1:101:A:LEU:H | 1:100:A:GLU:H   | 22       | 0.1           |
| (1,111) | 1:63:A:CYS:H  | 1:60:A:ASP:H    | 10       | 0.1           |
| (1,55)  | 1:42:A:TRP:H  | 1:42:A:TRP:HB3  | 9        | 0.1           |

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| Key    | Atom-1       | Atom-2         | Model ID | Violation (Å) |
|--------|--------------|----------------|----------|---------------|
| (1,55) | 1:42:A:TRP:H | 1:42:A:TRP:HB3 | 11       | 0.1           |
| (1,55) | 1:42:A:TRP:H | 1:42:A:TRP:HB3 | 13       | 0.1           |
| (1,55) | 1:42:A:TRP:H | 1:42:A:TRP:HB3 | 15       | 0.1           |
| (1,55) | 1:42:A:TRP:H | 1:42:A:TRP:HB3 | 26       | 0.1           |
| (1,55) | 1:42:A:TRP:H | 1:42:A:TRP:HB3 | 28       | 0.1           |
| (1,55) | 1:42:A:TRP:H | 1:42:A:TRP:HB3 | 32       | 0.1           |
| (1,55) | 1:42:A:TRP:H | 1:42:A:TRP:HB3 | 35       | 0.1           |
| (1,24) | 1:89:A:GLY:H | 1:9:A:PRO:HB3  | 6        | 0.1           |

## 10 Dihedral-angle violation analysis [i](#)

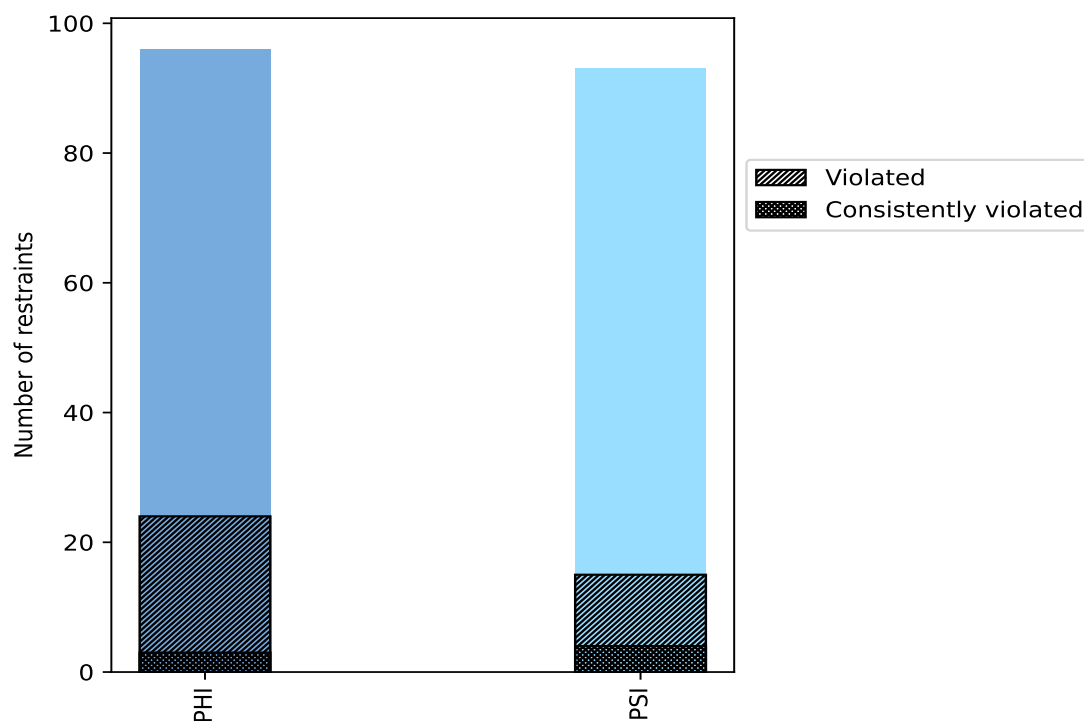
### 10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PHI        | 96    | 50.8           | 24                    | 25.0           | 12.7           | 3                                  | 3.1            | 1.6            |
| PSI        | 93    | 49.2           | 15                    | 16.1           | 7.9            | 4                                  | 4.3            | 2.1            |
| Total      | 189   | 100.0          | 39                    | 20.6           | 20.6           | 7                                  | 3.7            | 3.7            |

<sup>1</sup> percentage calculated with respect to total number of dihedral-angle restraints, <sup>2</sup> percentage calculated with respect to number of restraints in a particular dihedral-angle type, <sup>3</sup> violated in at least one model, <sup>4</sup> violated in all the models

#### 10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PHI                  | PSI | Total |          |         |        |            |
| 1        | 15                   | 10  | 25    | 2.66     | 4.88    | 1.16   | 2.28       |
| 2        | 16                   | 12  | 28    | 2.35     | 4.77    | 1.02   | 2.15       |
| 3        | 12                   | 10  | 22    | 2.65     | 6.1     | 1.35   | 2.32       |
| 4        | 16                   | 11  | 27    | 2.5      | 4.91    | 1.02   | 2.42       |
| 5        | 13                   | 10  | 23    | 2.3      | 4.96    | 1.07   | 2.19       |
| 6        | 13                   | 10  | 23    | 2.33     | 5.31    | 1.2    | 1.93       |
| 7        | 15                   | 9   | 24    | 2.45     | 4.86    | 0.92   | 2.28       |
| 8        | 13                   | 11  | 24    | 2.66     | 5.31    | 1.13   | 2.3        |
| 9        | 13                   | 9   | 22    | 2.49     | 4.8     | 1.08   | 2.12       |
| 10       | 15                   | 11  | 26    | 2.42     | 4.93    | 1.17   | 2.41       |
| 11       | 12                   | 9   | 21    | 2.39     | 4.42    | 0.92   | 2.18       |
| 12       | 12                   | 10  | 22    | 2.56     | 5.01    | 1.12   | 2.18       |
| 13       | 12                   | 11  | 23    | 2.65     | 4.95    | 1.07   | 2.46       |
| 14       | 15                   | 12  | 27    | 2.51     | 6.09    | 1.24   | 2.34       |
| 15       | 13                   | 11  | 24    | 2.55     | 5.01    | 1.07   | 2.22       |
| 16       | 15                   | 10  | 25    | 2.5      | 5.98    | 1.23   | 2.14       |
| 17       | 11                   | 8   | 19    | 2.65     | 5.92    | 1.21   | 2.38       |
| 18       | 14                   | 10  | 24    | 2.61     | 5.44    | 1.12   | 2.22       |
| 19       | 14                   | 10  | 24    | 2.56     | 5.98    | 1.46   | 2.22       |
| 20       | 13                   | 11  | 24    | 2.53     | 5.06    | 1.2    | 1.99       |
| 21       | 11                   | 11  | 22    | 2.09     | 3.75    | 0.72   | 2.12       |
| 22       | 9                    | 10  | 19    | 2.06     | 3.48    | 0.68   | 2.03       |
| 23       | 12                   | 11  | 23    | 2.12     | 3.4     | 0.69   | 2.13       |
| 24       | 11                   | 10  | 21    | 2.25     | 4.64    | 0.91   | 2.02       |
| 25       | 12                   | 10  | 22    | 1.91     | 3.2     | 0.63   | 1.92       |
| 26       | 13                   | 9   | 22    | 2.33     | 5.16    | 0.88   | 2.0        |
| 27       | 12                   | 10  | 22    | 2.31     | 5.79    | 1.09   | 2.24       |
| 28       | 16                   | 11  | 27    | 2.04     | 5.11    | 0.94   | 1.79       |
| 29       | 15                   | 8   | 23    | 2.45     | 5.28    | 1.04   | 2.31       |
| 30       | 14                   | 10  | 24    | 2.18     | 5.13    | 0.91   | 2.04       |
| 31       | 13                   | 11  | 24    | 2.21     | 5.12    | 0.91   | 2.06       |
| 32       | 13                   | 10  | 23    | 2.09     | 4.1     | 0.79   | 2.07       |
| 33       | 14                   | 11  | 25    | 2.35     | 5.16    | 0.88   | 2.1        |
| 34       | 12                   | 9   | 21    | 2.03     | 3.8     | 0.82   | 1.71       |
| 35       | 15                   | 10  | 25    | 1.97     | 3.62    | 0.75   | 1.82       |
| 36       | 14                   | 10  | 24    | 2.12     | 3.8     | 0.77   | 2.14       |
| 37       | 14                   | 9   | 23    | 2.1      | 3.47    | 0.66   | 2.12       |
| 38       | 13                   | 11  | 24    | 2.13     | 5.23    | 0.94   | 1.94       |

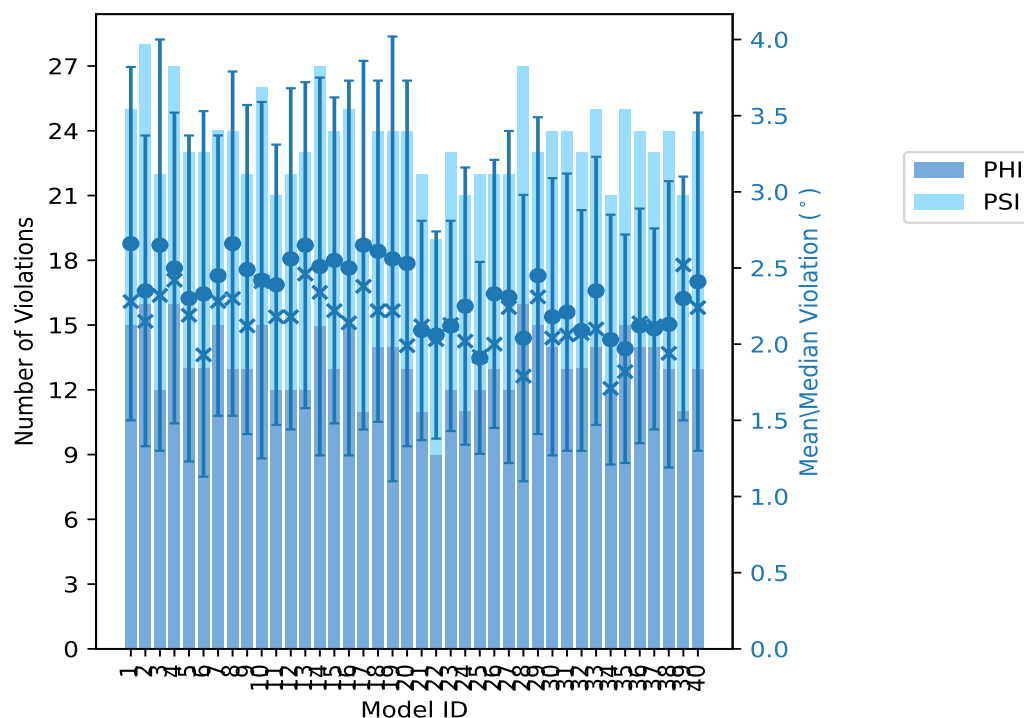
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| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PHI                  | PSI | Total |          |         |        |            |
| 39       | 11                   | 10  | 21    | 2.3      | 3.5     | 0.8    | 2.52       |
| 40       | 13                   | 11  | 24    | 2.41     | 5.49    | 1.11   | 2.24       |

### 10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



The mean(dot), median(x) and the standard deviation are shown in blue with respect to the y axis on the right

### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

| Number of violated restraints |     |       | Fraction of the ensemble |      |
|-------------------------------|-----|-------|--------------------------|------|
| PHI                           | PSI | Total | Count <sup>1</sup>       | %    |
| 3                             | 2   | 5     | 1                        | 2.5  |
| 2                             | 0   | 2     | 2                        | 5.0  |
| 0                             | 0   | 0     | 3                        | 7.5  |
| 0                             | 0   | 0     | 4                        | 10.0 |

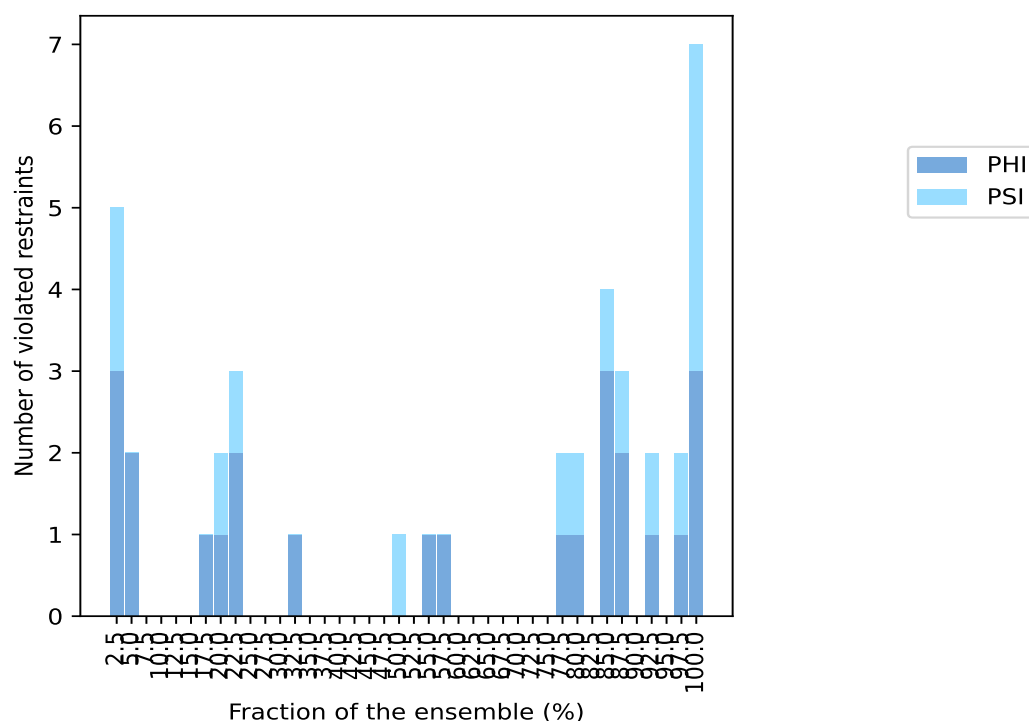
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PHI                           | PSI | Total | Count <sup>1</sup>       | %     |
| 0                             | 0   | 0     | 5                        | 12.5  |
| 0                             | 0   | 0     | 6                        | 15.0  |
| 1                             | 0   | 1     | 7                        | 17.5  |
| 1                             | 1   | 2     | 8                        | 20.0  |
| 2                             | 1   | 3     | 9                        | 22.5  |
| 0                             | 0   | 0     | 10                       | 25.0  |
| 0                             | 0   | 0     | 11                       | 27.5  |
| 0                             | 0   | 0     | 12                       | 30.0  |
| 1                             | 0   | 1     | 13                       | 32.5  |
| 0                             | 0   | 0     | 14                       | 35.0  |
| 0                             | 0   | 0     | 15                       | 37.5  |
| 0                             | 0   | 0     | 16                       | 40.0  |
| 0                             | 0   | 0     | 17                       | 42.5  |
| 0                             | 0   | 0     | 18                       | 45.0  |
| 0                             | 0   | 0     | 19                       | 47.5  |
| 0                             | 1   | 1     | 20                       | 50.0  |
| 0                             | 0   | 0     | 21                       | 52.5  |
| 1                             | 0   | 1     | 22                       | 55.0  |
| 1                             | 0   | 1     | 23                       | 57.5  |
| 0                             | 0   | 0     | 24                       | 60.0  |
| 0                             | 0   | 0     | 25                       | 62.5  |
| 0                             | 0   | 0     | 26                       | 65.0  |
| 0                             | 0   | 0     | 27                       | 67.5  |
| 0                             | 0   | 0     | 28                       | 70.0  |
| 0                             | 0   | 0     | 29                       | 72.5  |
| 0                             | 0   | 0     | 30                       | 75.0  |
| 1                             | 1   | 2     | 31                       | 77.5  |
| 1                             | 1   | 2     | 32                       | 80.0  |
| 0                             | 0   | 0     | 33                       | 82.5  |
| 3                             | 1   | 4     | 34                       | 85.0  |
| 2                             | 1   | 3     | 35                       | 87.5  |
| 0                             | 0   | 0     | 36                       | 90.0  |
| 1                             | 1   | 2     | 37                       | 92.5  |
| 0                             | 0   | 0     | 38                       | 95.0  |
| 1                             | 1   | 2     | 39                       | 97.5  |
| 3                             | 4   | 7     | 40                       | 100.0 |

<sup>1</sup> Number of models with violations

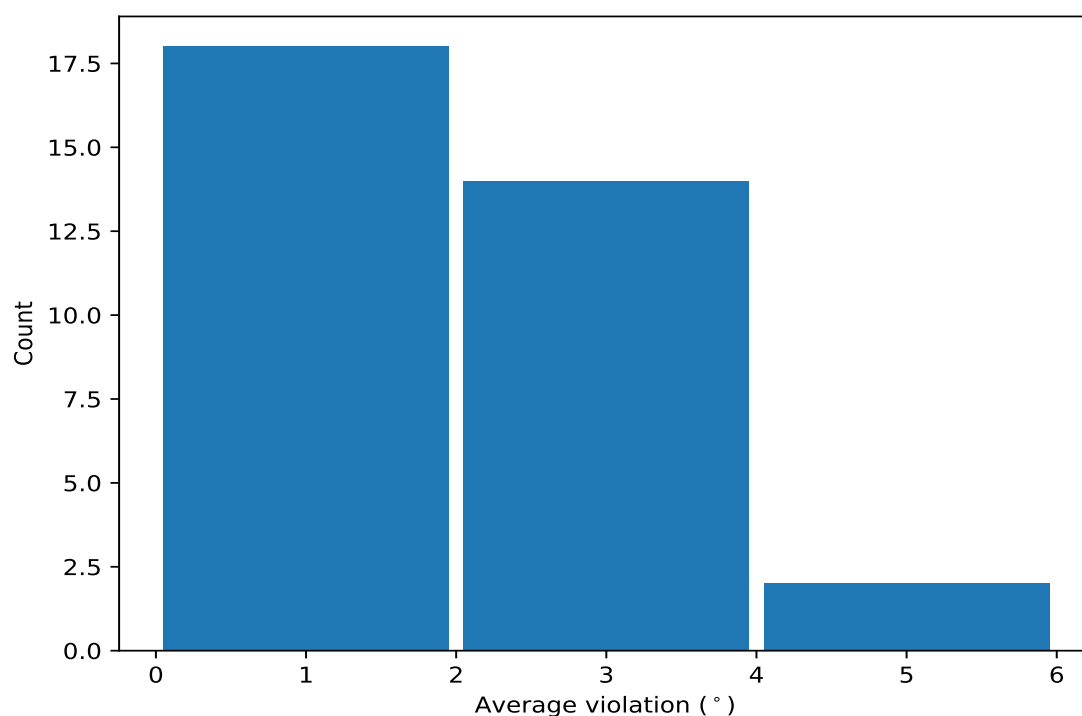
### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

### 10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



#### 10.4.2 Table: Most violated dihedral-angle restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 40                  | 3.48 | 0.38            | 3.48   |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 40                  | 3.22 | 0.57            | 3.22   |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 40                  | 2.64 | 0.67            | 2.56   |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 40                  | 2.57 | 0.42            | 2.53   |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 40                  | 2.34 | 0.27            | 2.37   |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 40                  | 2.17 | 0.28            | 2.16   |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 40                  | 2.17 | 0.37            | 2.17   |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 39                  | 2.31 | 0.59            | 2.37   |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 39                  | 1.68 | 0.41            | 1.57   |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 37                  | 3.24 | 0.52            | 3.16   |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 37                  | 1.63 | 0.29            | 1.66   |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 35                  | 2.6  | 0.65            | 2.76   |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 35                  | 1.79 | 0.5             | 1.78   |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 35                  | 1.3  | 0.16            | 1.27   |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 34                  | 3.84 | 1.59            | 4.62   |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 34                  | 2.3  | 0.26            | 2.29   |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 34                  | 1.85 | 0.56            | 1.72   |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 34                  | 1.42 | 0.25            | 1.38   |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 32                  | 2.14 | 0.78            | 2.15   |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 32                  | 1.88 | 0.32            | 1.9    |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 31                  | 2.58 | 1.2             | 2.59   |

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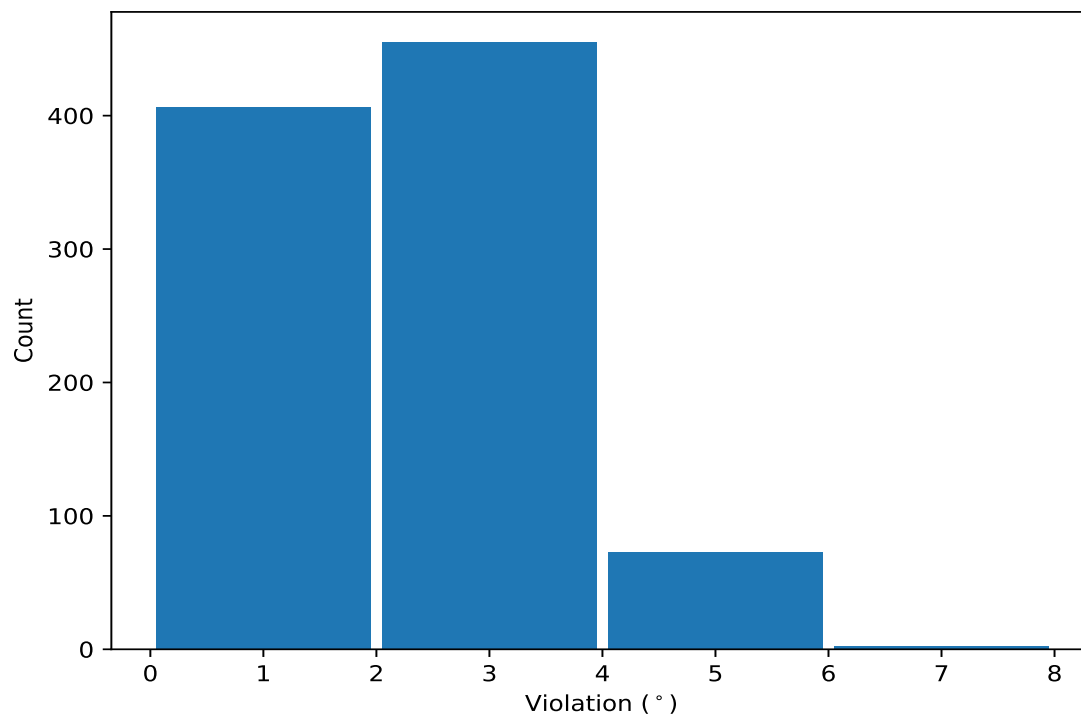
| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 31                  | 1.58 | 0.31            | 1.55   |
| (1,128) | 1:71:A:VAL:C | 1:72:A:THR:N  | 1:72:A:THR:CA | 1:72:A:THR:C | 23                  | 1.52 | 0.4             | 1.38   |
| (1,154) | 1:85:A:LEU:C | 1:86:A:GLU:N  | 1:86:A:GLU:CA | 1:86:A:GLU:C | 22                  | 4.58 | 1.13            | 4.84   |
| (1,153) | 1:85:A:LEU:N | 1:85:A:LEU:CA | 1:85:A:LEU:C  | 1:86:A:GLU:N | 20                  | 4.97 | 0.56            | 4.86   |
| (1,57)  | 1:34:A:SER:C | 1:35:A:PHE:N  | 1:35:A:PHE:CA | 1:35:A:PHE:C | 13                  | 1.79 | 0.37            | 1.84   |
| (1,152) | 1:84:A:ARG:C | 1:85:A:LEU:N  | 1:85:A:LEU:CA | 1:85:A:LEU:C | 9                   | 1.68 | 0.38            | 1.68   |
| (1,126) | 1:70:A:ASN:C | 1:71:A:VAL:N  | 1:71:A:VAL:CA | 1:71:A:VAL:C | 9                   | 1.28 | 0.32            | 1.14   |
| (1,109) | 1:62:A:ARG:N | 1:62:A:ARG:CA | 1:62:A:ARG:C  | 1:63:A:CYS:N | 9                   | 1.2  | 0.14            | 1.2    |
| (1,59)  | 1:35:A:PHE:C | 1:36:A:ASP:N  | 1:36:A:ASP:CA | 1:36:A:ASP:C | 8                   | 1.82 | 0.57            | 1.78   |
| (1,157) | 1:87:A:PRO:N | 1:87:A:PRO:CA | 1:87:A:PRO:C  | 1:88:A:ARG:N | 8                   | 1.13 | 0.13            | 1.06   |
| (1,19)  | 1:14:A:LYS:C | 1:15:A:ARG:N  | 1:15:A:ARG:CA | 1:15:A:ARG:C | 7                   | 1.11 | 0.08            | 1.14   |
| (1,112) | 1:63:A:CYS:C | 1:64:A:HIS:N  | 1:64:A:HIS:CA | 1:64:A:HIS:C | 2                   | 1.41 | 0.2             | 1.41   |
| (1,108) | 1:61:A:GLY:C | 1:62:A:ARG:N  | 1:62:A:ARG:CA | 1:62:A:ARG:C | 2                   | 1.12 | 0.08            | 1.12   |

<sup>1</sup> Number of violated models, <sup>2</sup>Standard deviation, All angle values are in degree (°)

## 10.5 All violated dihedral-angle restraints [i](#)

### 10.5.1 Histogram : Distribution of violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



### 10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,153) | 1:85:A:LEU:N | 1:85:A:LEU:CA | 1:85:A:LEU:C  | 1:86:A:GLU:N | 3        | 6.1           |
| (1,154) | 1:85:A:LEU:C | 1:86:A:GLU:N  | 1:86:A:GLU:CA | 1:86:A:GLU:C | 14       | 6.09          |
| (1,153) | 1:85:A:LEU:N | 1:85:A:LEU:CA | 1:85:A:LEU:C  | 1:86:A:GLU:N | 16       | 5.98          |
| (1,153) | 1:85:A:LEU:N | 1:85:A:LEU:CA | 1:85:A:LEU:C  | 1:86:A:GLU:N | 19       | 5.98          |
| (1,154) | 1:85:A:LEU:C | 1:86:A:GLU:N  | 1:86:A:GLU:CA | 1:86:A:GLU:C | 17       | 5.92          |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 27       | 5.79          |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 3        | 5.7           |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 19       | 5.66          |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 40       | 5.49          |
| (1,154) | 1:85:A:LEU:C | 1:86:A:GLU:N  | 1:86:A:GLU:CA | 1:86:A:GLU:C | 18       | 5.44          |
| (1,153) | 1:85:A:LEU:N | 1:85:A:LEU:CA | 1:85:A:LEU:C  | 1:86:A:GLU:N | 14       | 5.34          |
| (1,153) | 1:85:A:LEU:N | 1:85:A:LEU:CA | 1:85:A:LEU:C  | 1:86:A:GLU:N | 8        | 5.31          |
| (1,153) | 1:85:A:LEU:N | 1:85:A:LEU:CA | 1:85:A:LEU:C  | 1:86:A:GLU:N | 17       | 5.31          |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 6        | 5.31          |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 29       | 5.28          |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 38       | 5.23          |
| (1,154) | 1:85:A:LEU:C | 1:86:A:GLU:N  | 1:86:A:GLU:CA | 1:86:A:GLU:C | 16       | 5.2           |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 26       | 5.16          |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 33       | 5.16          |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 30       | 5.13          |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 31       | 5.12          |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 28       | 5.11          |
| (1,153) | 1:85:A:LEU:N | 1:85:A:LEU:CA | 1:85:A:LEU:C  | 1:86:A:GLU:N | 20       | 5.06          |
| (1,154) | 1:85:A:LEU:C | 1:86:A:GLU:N  | 1:86:A:GLU:CA | 1:86:A:GLU:C | 19       | 5.03          |
| (1,154) | 1:85:A:LEU:C | 1:86:A:GLU:N  | 1:86:A:GLU:CA | 1:86:A:GLU:C | 6        | 5.02          |
| (1,154) | 1:85:A:LEU:C | 1:86:A:GLU:N  | 1:86:A:GLU:CA | 1:86:A:GLU:C | 12       | 5.01          |
| (1,153) | 1:85:A:LEU:N | 1:85:A:LEU:CA | 1:85:A:LEU:C  | 1:86:A:GLU:N | 15       | 5.01          |
| (1,153) | 1:85:A:LEU:N | 1:85:A:LEU:CA | 1:85:A:LEU:C  | 1:86:A:GLU:N | 5        | 4.96          |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 13       | 4.95          |
| (1,154) | 1:85:A:LEU:C | 1:86:A:GLU:N  | 1:86:A:GLU:CA | 1:86:A:GLU:C | 10       | 4.93          |
| (1,154) | 1:85:A:LEU:C | 1:86:A:GLU:N  | 1:86:A:GLU:CA | 1:86:A:GLU:C | 4        | 4.91          |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 1        | 4.88          |
| (1,153) | 1:85:A:LEU:N | 1:85:A:LEU:CA | 1:85:A:LEU:C  | 1:86:A:GLU:N | 10       | 4.87          |
| (1,154) | 1:85:A:LEU:C | 1:86:A:GLU:N  | 1:86:A:GLU:CA | 1:86:A:GLU:C | 7        | 4.86          |
| (1,154) | 1:85:A:LEU:C | 1:86:A:GLU:N  | 1:86:A:GLU:CA | 1:86:A:GLU:C | 8        | 4.86          |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 12       | 4.86          |
| (1,153) | 1:85:A:LEU:N | 1:85:A:LEU:CA | 1:85:A:LEU:C  | 1:86:A:GLU:N | 6        | 4.84          |
| (1,154) | 1:85:A:LEU:C | 1:86:A:GLU:N  | 1:86:A:GLU:CA | 1:86:A:GLU:C | 13       | 4.81          |
| (1,154) | 1:85:A:LEU:C | 1:86:A:GLU:N  | 1:86:A:GLU:CA | 1:86:A:GLU:C | 15       | 4.81          |
| (1,153) | 1:85:A:LEU:N | 1:85:A:LEU:CA | 1:85:A:LEU:C  | 1:86:A:GLU:N | 9        | 4.8           |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 14       | 4.79          |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 2        | 4.77          |
| (1,154) | 1:85:A:LEU:C | 1:86:A:GLU:N  | 1:86:A:GLU:CA | 1:86:A:GLU:C | 9        | 4.75          |
| (1,153) | 1:85:A:LEU:N | 1:85:A:LEU:CA | 1:85:A:LEU:C  | 1:86:A:GLU:N | 13       | 4.72          |
| (1,153) | 1:85:A:LEU:N | 1:85:A:LEU:CA | 1:85:A:LEU:C  | 1:86:A:GLU:N | 2        | 4.71          |
| (1,153) | 1:85:A:LEU:N | 1:85:A:LEU:CA | 1:85:A:LEU:C  | 1:86:A:GLU:N | 18       | 4.71          |
| (1,153) | 1:85:A:LEU:N | 1:85:A:LEU:CA | 1:85:A:LEU:C  | 1:86:A:GLU:N | 1        | 4.7           |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 20       | 4.68          |
| (1,154) | 1:85:A:LEU:C | 1:86:A:GLU:N  | 1:86:A:GLU:CA | 1:86:A:GLU:C | 1        | 4.68          |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 24       | 4.64          |
| (1,154) | 1:85:A:LEU:C | 1:86:A:GLU:N  | 1:86:A:GLU:CA | 1:86:A:GLU:C | 3        | 4.61          |
| (1,154) | 1:85:A:LEU:C | 1:86:A:GLU:N  | 1:86:A:GLU:CA | 1:86:A:GLU:C | 20       | 4.6           |
| (1,154) | 1:85:A:LEU:C | 1:86:A:GLU:N  | 1:86:A:GLU:CA | 1:86:A:GLU:C | 5        | 4.59          |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 10       | 4.59          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 19       | 4.59          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 18       | 4.52          |
| (1,153) | 1:85:A:LEU:N | 1:85:A:LEU:CA | 1:85:A:LEU:C  | 1:86:A:GLU:N | 12       | 4.49          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 40       | 4.47          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 4        | 4.46          |
| (1,154) | 1:85:A:LEU:C | 1:86:A:GLU:N  | 1:86:A:GLU:CA | 1:86:A:GLU:C | 11       | 4.42          |
| (1,153) | 1:85:A:LEU:N | 1:85:A:LEU:CA | 1:85:A:LEU:C  | 1:86:A:GLU:N | 11       | 4.41          |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 29       | 4.23          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 20       | 4.23          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 1        | 4.21          |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 20       | 4.2           |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 13       | 4.19          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 16       | 4.14          |
| (1,153) | 1:85:A:LEU:N | 1:85:A:LEU:CA | 1:85:A:LEU:C  | 1:86:A:GLU:N | 7        | 4.13          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 32       | 4.1           |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 11       | 4.09          |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 4        | 4.07          |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 16       | 4.06          |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 8        | 4.04          |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 10       | 4.04          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 8        | 4.01          |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 5        | 3.99          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 18       | 3.99          |
| (1,153) | 1:85:A:LEU:N | 1:85:A:LEU:CA | 1:85:A:LEU:C  | 1:86:A:GLU:N | 4        | 3.97          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 10       | 3.97          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 9        | 3.91          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 40       | 3.89          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 27       | 3.89          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 19       | 3.88          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 1        | 3.86          |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 1        | 3.81          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 34       | 3.8           |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 32       | 3.8           |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 36       | 3.8           |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 7        | 3.79          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 8        | 3.78          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 15       | 3.78          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 24       | 3.78          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 40       | 3.77          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 36       | 3.76          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 21       | 3.75          |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 9        | 3.74          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 12       | 3.74          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 29       | 3.73          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 1        | 3.72          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 17       | 3.72          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 1        | 3.71          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 14       | 3.7           |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 2        | 3.67          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 9        | 3.66          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 15       | 3.64          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 33       | 3.63          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 8        | 3.62          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 35       | 3.62          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 2        | 3.6           |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 18       | 3.57          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 40       | 3.57          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 13       | 3.56          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 15       | 3.56          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 30       | 3.56          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 15       | 3.54          |
| (1,154) | 1:85:A:LEU:C | 1:86:A:GLU:N  | 1:86:A:GLU:CA | 1:86:A:GLU:C | 2        | 3.53          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 4        | 3.53          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 19       | 3.53          |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 18       | 3.52          |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 15       | 3.52          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 2        | 3.51          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 4        | 3.51          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 2        | 3.51          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 12       | 3.5           |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 39       | 3.5           |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 26       | 3.49          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 26       | 3.48          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 22       | 3.48          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 37       | 3.47          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 14       | 3.47          |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 16       | 3.46          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 39       | 3.46          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 5        | 3.45          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 20       | 3.45          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 33       | 3.44          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 4        | 3.43          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 3        | 3.42          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 34       | 3.42          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 24       | 3.41          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 31       | 3.41          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 27       | 3.4           |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 23       | 3.4           |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 3        | 3.39          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 28       | 3.38          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 29       | 3.38          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 8        | 3.38          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 35       | 3.37          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 20       | 3.36          |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 7        | 3.34          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 12       | 3.34          |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 3        | 3.31          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 9        | 3.31          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 27       | 3.31          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 29       | 3.31          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 28       | 3.29          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 6        | 3.28          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 11       | 3.28          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 38       | 3.27          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 39       | 3.26          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 24       | 3.24          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 9        | 3.24          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 29       | 3.23          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 28       | 3.23          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 17       | 3.21          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 23       | 3.21          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 39       | 3.21          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 31       | 3.21          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 34       | 3.21          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 17       | 3.21          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 21       | 3.2           |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 25       | 3.2           |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 37       | 3.17          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 23       | 3.16          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 35       | 3.16          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 3        | 3.15          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 7        | 3.15          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 16       | 3.14          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 16       | 3.12          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 13       | 3.11          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 32       | 3.11          |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 6        | 3.1           |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 21       | 3.1           |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 34       | 3.09          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 38       | 3.09          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 31       | 3.08          |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 26       | 3.08          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 38       | 3.08          |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 23       | 3.06          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 8        | 3.06          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 18       | 3.06          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 8        | 3.06          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 23       | 3.05          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 25       | 3.05          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 31       | 3.04          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 30       | 3.04          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 33       | 3.04          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 7        | 3.03          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 21       | 3.02          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 3        | 3.02          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 14       | 3.02          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 37       | 3.01          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 19       | 3.01          |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 33       | 3.0           |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 30       | 3.0           |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 33       | 3.0           |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 16       | 3.0           |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 7        | 2.99          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 29       | 2.99          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 5        | 2.99          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 39       | 2.98          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 18       | 2.98          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 33       | 2.97          |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 15       | 2.96          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 15       | 2.96          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 12       | 2.96          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 8        | 2.95          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 10       | 2.94          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 36       | 2.94          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 38       | 2.94          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 28       | 2.93          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 29       | 2.91          |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 39       | 2.91          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 40       | 2.9           |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 3        | 2.89          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 40       | 2.89          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 27       | 2.88          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 24       | 2.88          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 30       | 2.88          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 22       | 2.88          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 35       | 2.87          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 14       | 2.87          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 39       | 2.87          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 35       | 2.86          |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 17       | 2.85          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 36       | 2.85          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 17       | 2.84          |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 36       | 2.83          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 11       | 2.82          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 4        | 2.82          |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 22       | 2.81          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 7        | 2.81          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 32       | 2.79          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 33       | 2.78          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 27       | 2.78          |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 37       | 2.77          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 1        | 2.77          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 30       | 2.77          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 24       | 2.77          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 22       | 2.76          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 26       | 2.76          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 10       | 2.76          |

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Continued from previous page...

| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 37       | 2.76          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 27       | 2.75          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 40       | 2.74          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 20       | 2.74          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 5        | 2.73          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 25       | 2.72          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 4        | 2.71          |
| (1,59)  | 1:35:A:PHE:C | 1:36:A:ASP:N  | 1:36:A:ASP:CA | 1:36:A:ASP:C | 29       | 2.7           |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 18       | 2.7           |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 34       | 2.69          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 20       | 2.69          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 5        | 2.68          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 36       | 2.68          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 14       | 2.68          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 19       | 2.68          |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 18       | 2.67          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 22       | 2.67          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 2        | 2.66          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 15       | 2.66          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 31       | 2.66          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 1        | 2.66          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 26       | 2.66          |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 31       | 2.65          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 13       | 2.65          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 32       | 2.65          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 13       | 2.64          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 14       | 2.64          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 28       | 2.64          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 39       | 2.64          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 28       | 2.64          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 36       | 2.64          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 38       | 2.63          |
| (1,57)  | 1:34:A:SER:C | 1:35:A:PHE:N  | 1:35:A:PHE:CA | 1:35:A:PHE:C | 4        | 2.63          |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 26       | 2.62          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 10       | 2.62          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 26       | 2.62          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 10       | 2.62          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 7        | 2.62          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 31       | 2.61          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 9        | 2.61          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 16       | 2.61          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 6        | 2.6           |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 19       | 2.6           |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 5        | 2.59          |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 37       | 2.59          |
| (1,128) | 1:71:A:VAL:C | 1:72:A:THR:N  | 1:72:A:THR:CA | 1:72:A:THR:C | 4        | 2.59          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 27       | 2.59          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 12       | 2.58          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 14       | 2.58          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 17       | 2.58          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 34       | 2.58          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 11       | 2.56          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 22       | 2.56          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 20       | 2.56          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 39       | 2.55          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 28       | 2.54          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 21       | 2.54          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 35       | 2.54          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 30       | 2.54          |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 14       | 2.53          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 39       | 2.53          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 4        | 2.53          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 38       | 2.53          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 1        | 2.53          |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 39       | 2.52          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 3        | 2.52          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 6        | 2.52          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 36       | 2.52          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 13       | 2.51          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 30       | 2.51          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 26       | 2.51          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 14       | 2.51          |
| (1,20)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:ILE:N | 37       | 2.51          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 22       | 2.51          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 23       | 2.51          |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 10       | 2.5           |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 14       | 2.5           |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 2        | 2.49          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 23       | 2.49          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 10       | 2.49          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 25       | 2.48          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 13       | 2.48          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 33       | 2.47          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 13       | 2.47          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 10       | 2.47          |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 38       | 2.46          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 13       | 2.46          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 30       | 2.46          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 35       | 2.45          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 7        | 2.45          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 40       | 2.45          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 33       | 2.45          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 8        | 2.44          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 4        | 2.44          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 2        | 2.43          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 12       | 2.43          |
| (1,56)  | 1:34:A:SER:N | 1:34:A:SER:CA | 1:34:A:SER:C  | 1:35:A:PHE:N | 11       | 2.43          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 24       | 2.43          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 17       | 2.43          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 24       | 2.43          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 27       | 2.43          |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 4        | 2.42          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 31       | 2.42          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 25       | 2.42          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 10       | 2.42          |
| (1,128) | 1:71:A:VAL:C | 1:72:A:THR:N  | 1:72:A:THR:CA | 1:72:A:THR:C | 7        | 2.41          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 3        | 2.41          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 38       | 2.41          |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 13       | 2.39          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 16       | 2.39          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 37       | 2.39          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 19       | 2.39          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 10       | 2.39          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 11       | 2.39          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 32       | 2.38          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 11       | 2.38          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 9        | 2.38          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 17       | 2.38          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 23       | 2.37          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 6        | 2.37          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 7        | 2.37          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 5        | 2.37          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 21       | 2.37          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 39       | 2.37          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 25       | 2.36          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 27       | 2.36          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 31       | 2.36          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 21       | 2.35          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 34       | 2.35          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 21       | 2.35          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 24       | 2.35          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 25       | 2.35          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 29       | 2.35          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 14       | 2.34          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 26       | 2.34          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 40       | 2.34          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 12       | 2.34          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 13       | 2.34          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 32       | 2.34          |
| (1,59)  | 1:35:A:PHE:C | 1:36:A:ASP:N  | 1:36:A:ASP:CA | 1:36:A:ASP:C | 1        | 2.33          |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 19       | 2.32          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 29       | 2.32          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 38       | 2.32          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 40       | 2.31          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 29       | 2.31          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 8        | 2.31          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 39       | 2.31          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 10       | 2.31          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 5        | 2.31          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 36       | 2.31          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 34       | 2.31          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 2        | 2.3           |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 21       | 2.3           |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 15       | 2.3           |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 21       | 2.3           |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 18       | 2.29          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 6        | 2.29          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 22       | 2.29          |
| (1,59)  | 1:35:A:PHE:C | 1:36:A:ASP:N  | 1:36:A:ASP:CA | 1:36:A:ASP:C | 40       | 2.29          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 22       | 2.29          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 36       | 2.29          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 23       | 2.29          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 14       | 2.29          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 35       | 2.29          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 8        | 2.29          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 32       | 2.28          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 1        | 2.28          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 37       | 2.28          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 19       | 2.27          |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 2        | 2.27          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 15       | 2.27          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 36       | 2.26          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 16       | 2.26          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 25       | 2.26          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 33       | 2.26          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 27       | 2.25          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 25       | 2.25          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 14       | 2.24          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 9        | 2.24          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 38       | 2.24          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 11       | 2.24          |
| (1,104) | 1:59:A:ASN:C | 1:60:A:ASP:N  | 1:60:A:ASP:CA | 1:60:A:ASP:C | 27       | 2.23          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 5        | 2.23          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 13       | 2.23          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 28       | 2.23          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 4        | 2.23          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 31       | 2.23          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 3        | 2.23          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 32       | 2.23          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 18       | 2.23          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 8        | 2.23          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 30       | 2.22          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 18       | 2.21          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 2        | 2.21          |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 2        | 2.2           |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 1        | 2.2           |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 12       | 2.2           |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 31       | 2.2           |
| (1,152) | 1:84:A:ARG:C | 1:85:A:LEU:N  | 1:85:A:LEU:CA | 1:85:A:LEU:C | 23       | 2.19          |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 28       | 2.19          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 7        | 2.19          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 5        | 2.19          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 29       | 2.19          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 40       | 2.19          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 16       | 2.19          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 37       | 2.19          |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 11       | 2.18          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 34       | 2.18          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 35       | 2.18          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 15       | 2.18          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 7        | 2.18          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 9        | 2.18          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 36       | 2.17          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 19       | 2.17          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 12       | 2.17          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 7        | 2.17          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 24       | 2.16          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 17       | 2.16          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 20       | 2.16          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 13       | 2.15          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 35       | 2.15          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 32       | 2.15          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 21       | 2.14          |
| (1,57)  | 1:34:A:SER:C | 1:35:A:PHE:N  | 1:35:A:PHE:CA | 1:35:A:PHE:C | 30       | 2.14          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 16       | 2.14          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 37       | 2.14          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 11       | 2.14          |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 23       | 2.13          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 23       | 2.13          |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 36       | 2.12          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 17       | 2.12          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 37       | 2.12          |
| (1,59)  | 1:35:A:PHE:C | 1:36:A:ASP:N  | 1:36:A:ASP:CA | 1:36:A:ASP:C | 18       | 2.12          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 39       | 2.12          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 33       | 2.12          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 21       | 2.11          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 33       | 2.1           |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 2        | 2.1           |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 4        | 2.09          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 16       | 2.09          |
| (1,126) | 1:70:A:ASN:C | 1:71:A:VAL:N  | 1:71:A:VAL:CA | 1:71:A:VAL:C | 7        | 2.08          |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 21       | 2.08          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 32       | 2.08          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 23       | 2.08          |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 1        | 2.07          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 32       | 2.07          |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 18       | 2.07          |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 11       | 2.07          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 12       | 2.07          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 30       | 2.06          |
| (1,152) | 1:84:A:ARG:C | 1:85:A:LEU:N  | 1:85:A:LEU:CA | 1:85:A:LEU:C | 28       | 2.06          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 19       | 2.06          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 9        | 2.06          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 35       | 2.06          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 28       | 2.06          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 2        | 2.06          |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 17       | 2.05          |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 25       | 2.05          |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 33       | 2.05          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 38       | 2.05          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 15       | 2.04          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 40       | 2.04          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 1        | 2.04          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 33       | 2.04          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 22       | 2.03          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 26       | 2.03          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 34       | 2.03          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 12       | 2.02          |
| (1,152) | 1:84:A:ARG:C | 1:85:A:LEU:N  | 1:85:A:LEU:CA | 1:85:A:LEU:C | 29       | 2.02          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 15       | 2.02          |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 30       | 2.02          |
| (1,57)  | 1:34:A:SER:C | 1:35:A:PHE:N  | 1:35:A:PHE:CA | 1:35:A:PHE:C | 20       | 2.02          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 24       | 2.02          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 16       | 2.02          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 33       | 2.02          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 29       | 2.01          |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 40       | 2.0           |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 19       | 2.0           |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 13       | 2.0           |
| (1,174) | 1:95:A:ALA:C | 1:96:A:GLU:N  | 1:96:A:GLU:CA | 1:96:A:GLU:C | 28       | 1.99          |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 11       | 1.99          |
| (1,128) | 1:71:A:VAL:C | 1:72:A:THR:N  | 1:72:A:THR:CA | 1:72:A:THR:C | 15       | 1.99          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 29       | 1.99          |
| (1,128) | 1:71:A:VAL:C | 1:72:A:THR:N  | 1:72:A:THR:CA | 1:72:A:THR:C | 6        | 1.98          |
| (1,57)  | 1:34:A:SER:C | 1:35:A:PHE:N  | 1:35:A:PHE:CA | 1:35:A:PHE:C | 9        | 1.98          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 30       | 1.98          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 30       | 1.98          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 37       | 1.97          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 5        | 1.97          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 6        | 1.97          |
| (1,152) | 1:84:A:ARG:C | 1:85:A:LEU:N  | 1:85:A:LEU:CA | 1:85:A:LEU:C | 35       | 1.96          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 17       | 1.96          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 20       | 1.96          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 26       | 1.96          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 8        | 1.95          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 25       | 1.95          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 2        | 1.94          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 1        | 1.94          |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 9        | 1.94          |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 26       | 1.94          |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 32       | 1.94          |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 8        | 1.94          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 18       | 1.94          |
| (1,57)  | 1:34:A:SER:C | 1:35:A:PHE:N  | 1:35:A:PHE:CA | 1:35:A:PHE:C | 18       | 1.94          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 14       | 1.93          |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 6        | 1.93          |

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Continued from previous page...

| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 7        | 1.93          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 3        | 1.93          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 31       | 1.92          |
| (1,63)  | 1:37:A:ASP:C | 1:38:A:ALA:N  | 1:38:A:ALA:CA | 1:38:A:ALA:C | 1        | 1.92          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 37       | 1.92          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 3        | 1.92          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 1        | 1.92          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 12       | 1.92          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 23       | 1.91          |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 13       | 1.9           |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 24       | 1.9           |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 37       | 1.9           |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 24       | 1.89          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 20       | 1.89          |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 8        | 1.89          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 31       | 1.89          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 26       | 1.88          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 25       | 1.88          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 24       | 1.88          |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 14       | 1.87          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 6        | 1.87          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 26       | 1.87          |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 33       | 1.86          |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 37       | 1.86          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 4        | 1.86          |
| (1,128) | 1:71:A:VAL:C | 1:72:A:THR:N  | 1:72:A:THR:CA | 1:72:A:THR:C | 26       | 1.85          |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 27       | 1.85          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 6        | 1.85          |
| (1,57)  | 1:34:A:SER:C | 1:35:A:PHE:N  | 1:35:A:PHE:CA | 1:35:A:PHE:C | 8        | 1.85          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 40       | 1.85          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 22       | 1.84          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 36       | 1.84          |
| (1,128) | 1:71:A:VAL:C | 1:72:A:THR:N  | 1:72:A:THR:CA | 1:72:A:THR:C | 12       | 1.84          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 2        | 1.84          |
| (1,57)  | 1:34:A:SER:C | 1:35:A:PHE:N  | 1:35:A:PHE:CA | 1:35:A:PHE:C | 33       | 1.84          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 10       | 1.83          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 38       | 1.83          |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 33       | 1.82          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 8        | 1.82          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 35       | 1.82          |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 22       | 1.81          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 32       | 1.81          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 20       | 1.81          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 18       | 1.81          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 11       | 1.81          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 36       | 1.81          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 8        | 1.8           |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 3        | 1.8           |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 26       | 1.8           |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 15       | 1.8           |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 31       | 1.8           |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 11       | 1.79          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 28       | 1.79          |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 13       | 1.79          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 16       | 1.79          |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 35       | 1.78          |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 21       | 1.78          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 38       | 1.78          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 28       | 1.78          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 37       | 1.78          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 9        | 1.77          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 4        | 1.77          |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 15       | 1.77          |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 27       | 1.77          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 4        | 1.77          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 5        | 1.77          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 20       | 1.76          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 19       | 1.76          |
| (1,33)  | 1:21:A:VAL:C | 1:22:A:SER:N  | 1:22:A:SER:CA | 1:22:A:SER:C | 31       | 1.76          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 6        | 1.75          |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 36       | 1.75          |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 22       | 1.75          |
| (1,57)  | 1:34:A:SER:C | 1:35:A:PHE:N  | 1:35:A:PHE:CA | 1:35:A:PHE:C | 2        | 1.75          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 17       | 1.75          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 33       | 1.75          |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 35       | 1.74          |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 16       | 1.74          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 10       | 1.74          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 39       | 1.74          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 26       | 1.74          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 6        | 1.73          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 27       | 1.72          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 28       | 1.71          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 12       | 1.71          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 34       | 1.71          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 29       | 1.7           |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 4        | 1.7           |
| (1,71)  | 1:41:A:THR:C | 1:42:A:TRP:N  | 1:42:A:TRP:CA | 1:42:A:TRP:C | 11       | 1.7           |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 23       | 1.7           |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 31       | 1.7           |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 5        | 1.69          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 2        | 1.69          |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 3        | 1.69          |
| (1,152) | 1:84:A:ARG:C | 1:85:A:LEU:N  | 1:85:A:LEU:CA | 1:85:A:LEU:C | 33       | 1.68          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 26       | 1.68          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 6        | 1.68          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 9        | 1.68          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 12       | 1.67          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 23       | 1.66          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 33       | 1.66          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 1        | 1.66          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 18       | 1.66          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 10       | 1.66          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 7        | 1.66          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 14       | 1.66          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 7        | 1.65          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 13       | 1.65          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 32       | 1.65          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 13       | 1.65          |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 32       | 1.64          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 3        | 1.63          |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 12       | 1.63          |
| (1,128) | 1:71:A:VAL:C | 1:72:A:THR:N  | 1:72:A:THR:CA | 1:72:A:THR:C | 38       | 1.62          |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 4        | 1.62          |
| (1,57)  | 1:34:A:SER:C | 1:35:A:PHE:N  | 1:35:A:PHE:CA | 1:35:A:PHE:C | 40       | 1.62          |
| (1,112) | 1:63:A:CYS:C | 1:64:A:HIS:N  | 1:64:A:HIS:CA | 1:64:A:HIS:C | 4        | 1.61          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 21       | 1.6           |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 8        | 1.6           |
| (1,126) | 1:70:A:ASN:C | 1:71:A:VAL:N  | 1:71:A:VAL:CA | 1:71:A:VAL:C | 37       | 1.6           |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 21       | 1.6           |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 16       | 1.59          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 20       | 1.59          |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 38       | 1.59          |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 7        | 1.59          |
| (1,22)  | 1:16:A:ILE:N | 1:16:A:ILE:CA | 1:16:A:ILE:C  | 1:17:A:GLN:N | 6        | 1.59          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 3        | 1.59          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 17       | 1.58          |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 18       | 1.58          |
| (1,57)  | 1:34:A:SER:C | 1:35:A:PHE:N  | 1:35:A:PHE:CA | 1:35:A:PHE:C | 1        | 1.58          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 24       | 1.57          |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 20       | 1.57          |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 40       | 1.57          |
| (1,57)  | 1:34:A:SER:C | 1:35:A:PHE:N  | 1:35:A:PHE:CA | 1:35:A:PHE:C | 34       | 1.57          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 11       | 1.57          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 19       | 1.57          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 23       | 1.57          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 14       | 1.56          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 38       | 1.56          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 40       | 1.56          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 32       | 1.56          |
| (1,154) | 1:85:A:LEU:C | 1:86:A:GLU:N  | 1:86:A:GLU:CA | 1:86:A:GLU:C | 29       | 1.55          |
| (1,152) | 1:84:A:ARG:C | 1:85:A:LEU:N  | 1:85:A:LEU:CA | 1:85:A:LEU:C | 36       | 1.55          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 22       | 1.55          |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 9        | 1.55          |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 4        | 1.54          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 9        | 1.54          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 5        | 1.54          |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 24       | 1.54          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 5        | 1.53          |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 23       | 1.53          |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 30       | 1.53          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 11       | 1.52          |
| (1,109) | 1:62:A:ARG:N | 1:62:A:ARG:CA | 1:62:A:ARG:C  | 1:63:A:CYS:N | 31       | 1.52          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 35       | 1.52          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 18       | 1.52          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 38       | 1.52          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 16       | 1.52          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 3        | 1.52          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 20       | 1.52          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 28       | 1.52          |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 20       | 1.51          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 9        | 1.51          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 16       | 1.5           |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 18       | 1.5           |
| (1,128) | 1:71:A:VAL:C | 1:72:A:THR:N  | 1:72:A:THR:CA | 1:72:A:THR:C | 36       | 1.5           |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 18       | 1.5           |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 15       | 1.49          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 12       | 1.49          |
| (1,58)  | 1:35:A:PHE:N | 1:35:A:PHE:CA | 1:35:A:PHE:C  | 1:36:A:ASP:N | 17       | 1.49          |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 36       | 1.48          |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 30       | 1.47          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 10       | 1.47          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 34       | 1.47          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 4        | 1.47          |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 15       | 1.47          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 7        | 1.47          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 15       | 1.47          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 38       | 1.47          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 27       | 1.46          |
| (1,128) | 1:71:A:VAL:C | 1:72:A:THR:N  | 1:72:A:THR:CA | 1:72:A:THR:C | 9        | 1.46          |
| (1,128) | 1:71:A:VAL:C | 1:72:A:THR:N  | 1:72:A:THR:CA | 1:72:A:THR:C | 16       | 1.46          |
| (1,18)  | 1:14:A:LYS:N | 1:14:A:LYS:CA | 1:14:A:LYS:C  | 1:15:A:ARG:N | 2        | 1.46          |
| (1,161) | 1:89:A:GLY:N | 1:89:A:GLY:CA | 1:89:A:GLY:C  | 1:90:A:GLU:N | 15       | 1.45          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 3        | 1.45          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 30       | 1.45          |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 34       | 1.45          |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 34       | 1.45          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 16       | 1.45          |
| (1,59)  | 1:35:A:PHE:C | 1:36:A:ASP:N  | 1:36:A:ASP:CA | 1:36:A:ASP:C | 7        | 1.45          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 17       | 1.44          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 19       | 1.44          |
| (1,59)  | 1:35:A:PHE:C | 1:36:A:ASP:N  | 1:36:A:ASP:CA | 1:36:A:ASP:C | 31       | 1.44          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 36       | 1.44          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 29       | 1.44          |
| (1,128) | 1:71:A:VAL:C | 1:72:A:THR:N  | 1:72:A:THR:CA | 1:72:A:THR:C | 20       | 1.43          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 30       | 1.43          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 28       | 1.43          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 2        | 1.43          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 14       | 1.43          |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 23       | 1.42          |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 39       | 1.42          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 27       | 1.41          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 30       | 1.41          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 14       | 1.41          |

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Continued from previous page...

| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 2        | 1.41          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 10       | 1.4           |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 4        | 1.4           |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 25       | 1.39          |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 2        | 1.38          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 32       | 1.38          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 14       | 1.38          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 25       | 1.38          |
| (1,128) | 1:71:A:VAL:C | 1:72:A:THR:N  | 1:72:A:THR:CA | 1:72:A:THR:C | 14       | 1.38          |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 25       | 1.38          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 23       | 1.38          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 25       | 1.38          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 35       | 1.38          |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 29       | 1.37          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 11       | 1.37          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 24       | 1.37          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 27       | 1.37          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 24       | 1.37          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 7        | 1.36          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 20       | 1.36          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 22       | 1.36          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 39       | 1.35          |
| (1,152) | 1:84:A:ARG:C | 1:85:A:LEU:N  | 1:85:A:LEU:CA | 1:85:A:LEU:C | 26       | 1.35          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 16       | 1.35          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 5        | 1.35          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 6        | 1.35          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 37       | 1.35          |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 24       | 1.34          |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 21       | 1.34          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 10       | 1.34          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 15       | 1.34          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 25       | 1.33          |
| (1,157) | 1:87:A:PRO:N | 1:87:A:PRO:CA | 1:87:A:PRO:C  | 1:88:A:ARG:N | 34       | 1.33          |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 9        | 1.33          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 21       | 1.33          |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 21       | 1.32          |
| (1,157) | 1:87:A:PRO:N | 1:87:A:PRO:CA | 1:87:A:PRO:C  | 1:88:A:ARG:N | 40       | 1.32          |
| (1,128) | 1:71:A:VAL:C | 1:72:A:THR:N  | 1:72:A:THR:CA | 1:72:A:THR:C | 5        | 1.32          |
| (1,128) | 1:71:A:VAL:C | 1:72:A:THR:N  | 1:72:A:THR:CA | 1:72:A:THR:C | 28       | 1.32          |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 1        | 1.32          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 5        | 1.32          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 20       | 1.31          |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 25       | 1.31          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 34       | 1.31          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 28       | 1.31          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 31       | 1.31          |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 31       | 1.3           |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 35       | 1.3           |
| (1,128) | 1:71:A:VAL:C | 1:72:A:THR:N  | 1:72:A:THR:CA | 1:72:A:THR:C | 21       | 1.3           |
| (1,109) | 1:62:A:ARG:N | 1:62:A:ARG:CA | 1:62:A:ARG:C  | 1:63:A:CYS:N | 8        | 1.3           |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 13       | 1.3           |

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Continued from previous page...

| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 16       | 1.3           |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 6        | 1.3           |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 30       | 1.29          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 31       | 1.29          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 23       | 1.29          |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 27       | 1.28          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 26       | 1.28          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 1        | 1.27          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 2        | 1.27          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 22       | 1.27          |
| (1,128) | 1:71:A:VAL:C | 1:72:A:THR:N  | 1:72:A:THR:CA | 1:72:A:THR:C | 2        | 1.26          |
| (1,109) | 1:62:A:ARG:N | 1:62:A:ARG:CA | 1:62:A:ARG:C  | 1:63:A:CYS:N | 2        | 1.26          |
| (1,57)  | 1:34:A:SER:C | 1:35:A:PHE:N  | 1:35:A:PHE:CA | 1:35:A:PHE:C | 32       | 1.26          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 17       | 1.26          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 25       | 1.26          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 40       | 1.26          |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 19       | 1.25          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 28       | 1.25          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 35       | 1.25          |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 32       | 1.25          |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 5        | 1.25          |
| (1,128) | 1:71:A:VAL:C | 1:72:A:THR:N  | 1:72:A:THR:CA | 1:72:A:THR:C | 25       | 1.24          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 15       | 1.24          |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 10       | 1.23          |
| (1,157) | 1:87:A:PRO:N | 1:87:A:PRO:CA | 1:87:A:PRO:C  | 1:88:A:ARG:N | 6        | 1.23          |
| (1,152) | 1:84:A:ARG:C | 1:85:A:LEU:N  | 1:85:A:LEU:CA | 1:85:A:LEU:C | 37       | 1.23          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 1        | 1.23          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 26       | 1.23          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 34       | 1.23          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 35       | 1.23          |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 25       | 1.22          |
| (1,128) | 1:71:A:VAL:C | 1:72:A:THR:N  | 1:72:A:THR:CA | 1:72:A:THR:C | 22       | 1.22          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 12       | 1.22          |
| (1,59)  | 1:35:A:PHE:C | 1:36:A:ASP:N  | 1:36:A:ASP:CA | 1:36:A:ASP:C | 8        | 1.22          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 35       | 1.21          |
| (1,128) | 1:71:A:VAL:C | 1:72:A:THR:N  | 1:72:A:THR:CA | 1:72:A:THR:C | 30       | 1.21          |
| (1,112) | 1:63:A:CYS:C | 1:64:A:HIS:N  | 1:64:A:HIS:CA | 1:64:A:HIS:C | 10       | 1.21          |
| (1,109) | 1:62:A:ARG:N | 1:62:A:ARG:CA | 1:62:A:ARG:C  | 1:63:A:CYS:N | 33       | 1.21          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 20       | 1.21          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 39       | 1.21          |
| (1,19)  | 1:14:A:LYS:C | 1:15:A:ARG:N  | 1:15:A:ARG:CA | 1:15:A:ARG:C | 33       | 1.21          |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 28       | 1.2           |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 32       | 1.2           |
| (1,128) | 1:71:A:VAL:C | 1:72:A:THR:N  | 1:72:A:THR:CA | 1:72:A:THR:C | 1        | 1.2           |
| (1,128) | 1:71:A:VAL:C | 1:72:A:THR:N  | 1:72:A:THR:CA | 1:72:A:THR:C | 32       | 1.2           |
| (1,109) | 1:62:A:ARG:N | 1:62:A:ARG:CA | 1:62:A:ARG:C  | 1:63:A:CYS:N | 14       | 1.2           |
| (1,108) | 1:61:A:GLY:C | 1:62:A:ARG:N  | 1:62:A:ARG:CA | 1:62:A:ARG:C | 14       | 1.2           |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 29       | 1.2           |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 29       | 1.2           |
| (1,154) | 1:85:A:LEU:C | 1:86:A:GLU:N  | 1:86:A:GLU:CA | 1:86:A:GLU:C | 28       | 1.19          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 24       | 1.19          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,19)  | 1:14:A:LYS:C | 1:15:A:ARG:N  | 1:15:A:ARG:CA | 1:15:A:ARG:C | 9        | 1.19          |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 40       | 1.18          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 4        | 1.18          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 39       | 1.17          |
| (1,126) | 1:70:A:ASN:C | 1:71:A:VAL:N  | 1:71:A:VAL:CA | 1:71:A:VAL:C | 4        | 1.17          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 37       | 1.16          |
| (1,103) | 1:59:A:ASN:N | 1:59:A:ASN:CA | 1:59:A:ASN:C  | 1:60:A:ASP:N | 38       | 1.16          |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 35       | 1.16          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 40       | 1.16          |
| (1,19)  | 1:14:A:LYS:C | 1:15:A:ARG:N  | 1:15:A:ARG:CA | 1:15:A:ARG:C | 30       | 1.16          |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 34       | 1.15          |
| (1,126) | 1:70:A:ASN:C | 1:71:A:VAL:N  | 1:71:A:VAL:CA | 1:71:A:VAL:C | 38       | 1.15          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 37       | 1.14          |
| (1,126) | 1:70:A:ASN:C | 1:71:A:VAL:N  | 1:71:A:VAL:CA | 1:71:A:VAL:C | 36       | 1.14          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 39       | 1.14          |
| (1,19)  | 1:14:A:LYS:C | 1:15:A:ARG:N  | 1:15:A:ARG:CA | 1:15:A:ARG:C | 38       | 1.14          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 10       | 1.14          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 18       | 1.14          |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 14       | 1.13          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 27       | 1.13          |
| (1,126) | 1:70:A:ASN:C | 1:71:A:VAL:N  | 1:71:A:VAL:CA | 1:71:A:VAL:C | 6        | 1.12          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 25       | 1.12          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 32       | 1.12          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 35       | 1.12          |
| (1,21)  | 1:15:A:ARG:C | 1:16:A:ILE:N  | 1:16:A:ILE:CA | 1:16:A:ILE:C | 22       | 1.12          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 27       | 1.12          |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 23       | 1.11          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 34       | 1.11          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 38       | 1.11          |
| (1,109) | 1:62:A:ARG:N | 1:62:A:ARG:CA | 1:62:A:ARG:C  | 1:63:A:CYS:N | 5        | 1.11          |
| (1,57)  | 1:34:A:SER:C | 1:35:A:PHE:N  | 1:35:A:PHE:CA | 1:35:A:PHE:C | 35       | 1.11          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 21       | 1.1           |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 33       | 1.1           |
| (1,128) | 1:71:A:VAL:C | 1:72:A:THR:N  | 1:72:A:THR:CA | 1:72:A:THR:C | 3        | 1.1           |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 34       | 1.1           |
| (1,126) | 1:70:A:ASN:C | 1:71:A:VAL:N  | 1:71:A:VAL:CA | 1:71:A:VAL:C | 16       | 1.09          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 27       | 1.08          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 28       | 1.08          |
| (1,152) | 1:84:A:ARG:C | 1:85:A:LEU:N  | 1:85:A:LEU:CA | 1:85:A:LEU:C | 40       | 1.08          |
| (1,126) | 1:70:A:ASN:C | 1:71:A:VAL:N  | 1:71:A:VAL:CA | 1:71:A:VAL:C | 10       | 1.08          |
| (1,126) | 1:70:A:ASN:C | 1:71:A:VAL:N  | 1:71:A:VAL:CA | 1:71:A:VAL:C | 31       | 1.08          |
| (1,109) | 1:62:A:ARG:N | 1:62:A:ARG:CA | 1:62:A:ARG:C  | 1:63:A:CYS:N | 23       | 1.08          |
| (1,92)  | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C  | 1:54:A:LYS:N | 36       | 1.08          |
| (1,83)  | 1:47:A:THR:C | 1:48:A:GLU:N  | 1:48:A:GLU:CA | 1:48:A:GLU:C | 36       | 1.08          |
| (1,109) | 1:62:A:ARG:N | 1:62:A:ARG:CA | 1:62:A:ARG:C  | 1:63:A:CYS:N | 12       | 1.07          |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 19       | 1.07          |
| (1,171) | 1:94:A:THR:N | 1:94:A:THR:CA | 1:94:A:THR:C  | 1:95:A:ALA:N | 28       | 1.06          |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 19       | 1.06          |
| (1,157) | 1:87:A:PRO:N | 1:87:A:PRO:CA | 1:87:A:PRO:C  | 1:88:A:ARG:N | 31       | 1.06          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 24       | 1.06          |
| (1,157) | 1:87:A:PRO:N | 1:87:A:PRO:CA | 1:87:A:PRO:C  | 1:88:A:ARG:N | 38       | 1.05          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,19)  | 1:14:A:LYS:C | 1:15:A:ARG:N  | 1:15:A:ARG:CA | 1:15:A:ARG:C | 5        | 1.05          |
| (1,162) | 1:89:A:GLY:C | 1:90:A:GLU:N  | 1:90:A:GLU:CA | 1:90:A:GLU:C | 7        | 1.04          |
| (1,128) | 1:71:A:VAL:C | 1:72:A:THR:N  | 1:72:A:THR:CA | 1:72:A:THR:C | 11       | 1.04          |
| (1,157) | 1:87:A:PRO:N | 1:87:A:PRO:CA | 1:87:A:PRO:C  | 1:88:A:ARG:N | 22       | 1.03          |
| (1,157) | 1:87:A:PRO:N | 1:87:A:PRO:CA | 1:87:A:PRO:C  | 1:88:A:ARG:N | 39       | 1.03          |
| (1,125) | 1:70:A:ASN:N | 1:70:A:ASN:CA | 1:70:A:ASN:C  | 1:71:A:VAL:N | 37       | 1.03          |
| (1,108) | 1:61:A:GLY:C | 1:62:A:ARG:N  | 1:62:A:ARG:CA | 1:62:A:ARG:C | 35       | 1.03          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 19       | 1.03          |
| (1,15)  | 1:12:A:PHE:C | 1:13:A:THR:N  | 1:13:A:THR:CA | 1:13:A:THR:C | 8        | 1.03          |
| (1,134) | 1:74:A:ASP:C | 1:75:A:ASP:N  | 1:75:A:ASP:CA | 1:75:A:ASP:C | 29       | 1.02          |
| (1,109) | 1:62:A:ARG:N | 1:62:A:ARG:CA | 1:62:A:ARG:C  | 1:63:A:CYS:N | 28       | 1.02          |
| (1,97)  | 1:56:A:ASN:N | 1:56:A:ASN:CA | 1:56:A:ASN:C  | 1:57:A:PHE:N | 36       | 1.02          |
| (1,45)  | 1:28:A:THR:C | 1:29:A:PHE:N  | 1:29:A:PHE:CA | 1:29:A:PHE:C | 13       | 1.02          |
| (1,19)  | 1:14:A:LYS:C | 1:15:A:ARG:N  | 1:15:A:ARG:CA | 1:15:A:ARG:C | 2        | 1.02          |
| (1,19)  | 1:14:A:LYS:C | 1:15:A:ARG:N  | 1:15:A:ARG:CA | 1:15:A:ARG:C | 3        | 1.02          |
| (1,5)   | 1:7:A:ALA:C  | 1:8:A:GLU:N   | 1:8:A:GLU:CA  | 1:8:A:GLU:C  | 19       | 1.02          |
| (1,160) | 1:88:A:ARG:C | 1:89:A:GLY:N  | 1:89:A:GLY:CA | 1:89:A:GLY:C | 28       | 1.01          |
| (1,158) | 1:87:A:PRO:C | 1:88:A:ARG:N  | 1:88:A:ARG:CA | 1:88:A:ARG:C | 6        | 1.01          |
| (1,157) | 1:87:A:PRO:N | 1:87:A:PRO:CA | 1:87:A:PRO:C  | 1:88:A:ARG:N | 21       | 1.01          |
| (1,84)  | 1:48:A:GLU:N | 1:48:A:GLU:CA | 1:48:A:GLU:C  | 1:49:A:LEU:N | 10       | 1.01          |
| (1,59)  | 1:35:A:PHE:C | 1:36:A:ASP:N  | 1:36:A:ASP:CA | 1:36:A:ASP:C | 30       | 1.01          |
| (1,25)  | 1:17:A:GLN:C | 1:18:A:ASN:N  | 1:18:A:ASN:CA | 1:18:A:ASN:C | 19       | 1.01          |