



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 03:31 AM UTC

PDB ID : 2LS7 / pdb\_00002ls7  
BMRB ID : 18412  
Title : High Definition Solution Structure of PED/PEA-15 Death Effector Domain  
Authors : Twomey, E.C.; Wei, Y.  
Deposited on : 2012-04-20

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

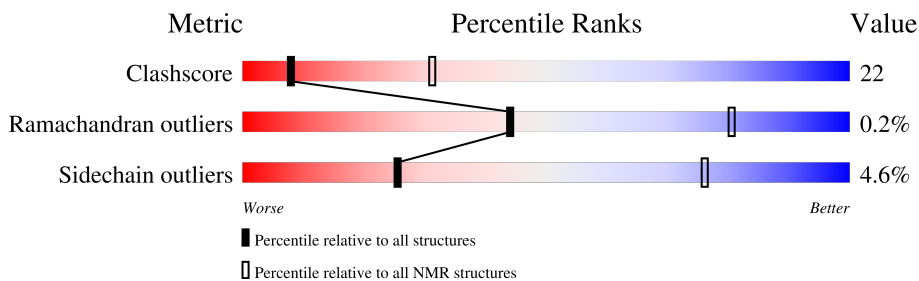
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 82%.

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     | 92     | 55% 37% . . .    |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:2-A:90 (89)         | 0.36              | 15           |

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 3 clusters and 11 single-model clusters were found.

| Cluster number        | Models                               |
|-----------------------|--------------------------------------|
| 1                     | 1, 5, 6, 11, 16                      |
| 2                     | 12, 15                               |
| 3                     | 14, 19                               |
| Single-model clusters | 2; 3; 4; 7; 8; 9; 10; 13; 17; 18; 20 |

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1458 atoms, of which 726 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Astrocytic phosphoprotein PEA-15.

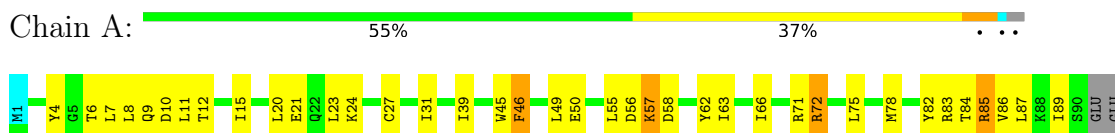
| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
|     |       |          | Total | C   | H   | N   | O   | S |       |
| 1   | A     | 90       | 1458  | 461 | 726 | 119 | 149 | 3 | 0     |

## 4 Residue-property plots [i](#)

### 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: Astrocytic phosphoprotein PEA-15

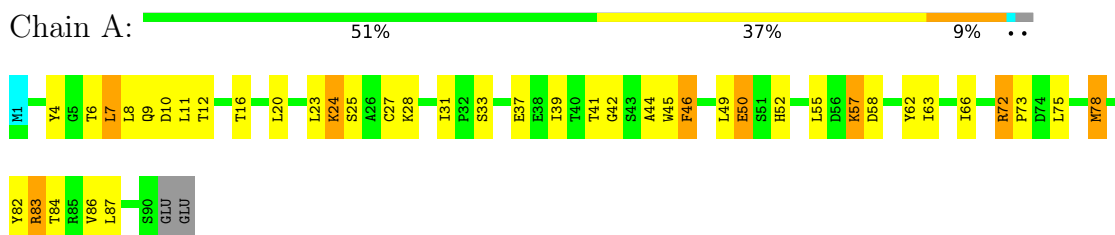


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

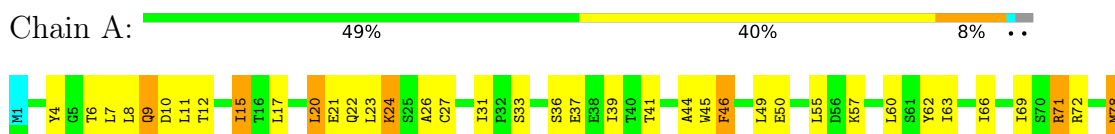
#### 4.2.1 Score per residue for model 1

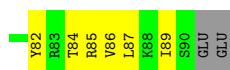
- Molecule 1: Astrocytic phosphoprotein PEA-15



#### 4.2.2 Score per residue for model 2

- Molecule 1: Astrocytic phosphoprotein PEA-15





### 4.2.3 Score per residue for model 3

- Molecule 1: Astrocytic phosphoprotein PEA-15

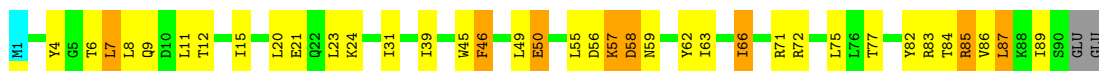
Chain A: 53% 28% 14% ...



### 4.2.4 Score per residue for model 4

- Molecule 1: Astrocytic phosphoprotein PEA-15

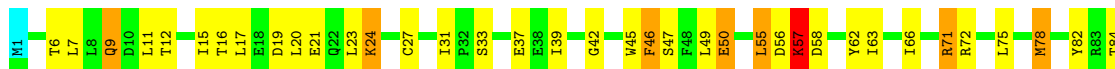
Chain A: 57% 32% 9% ..



### 4.2.5 Score per residue for model 5

- Molecule 1: Astrocytic phosphoprotein PEA-15

Chain A: 52% 35% 9% ...

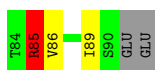


### 4.2.6 Score per residue for model 6

- Molecule 1: Astrocytic phosphoprotein PEA-15

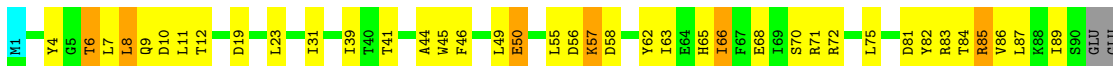
Chain A: 52% 36% 7% ...





#### 4.2.7 Score per residue for model 7

- Molecule 1: Astrocytic phosphoprotein PEA-15



#### 4.2.8 Score per residue for model 8

- Molecule 1: Astrocytic phosphoprotein PEA-15



#### 4.2.9 Score per residue for model 9

- Molecule 1: Astrocytic phosphoprotein PEA-15



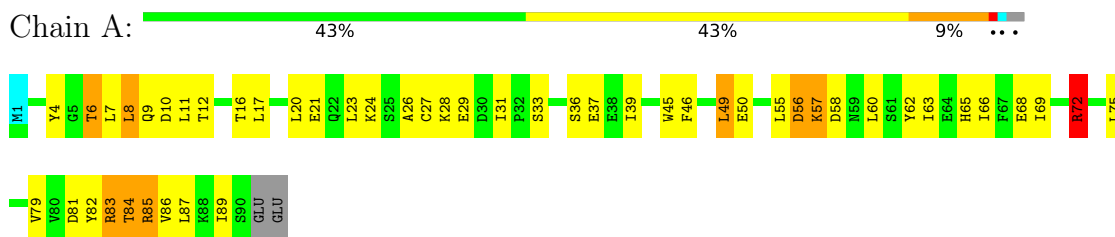
#### 4.2.10 Score per residue for model 10

- Molecule 1: Astrocytic phosphoprotein PEA-15



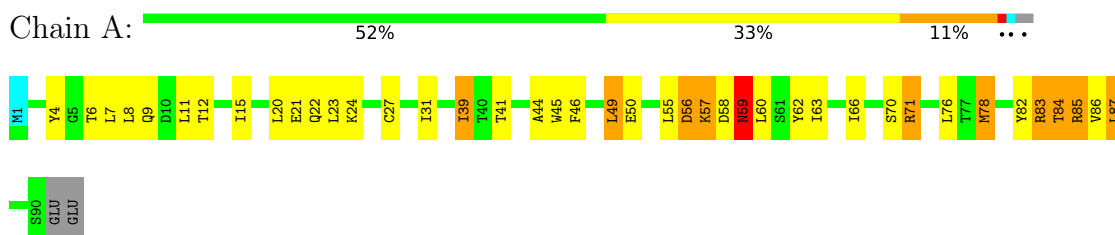
### 4.2.11 Score per residue for model 11

- Molecule 1: Astrocytic phosphoprotein PEA-15



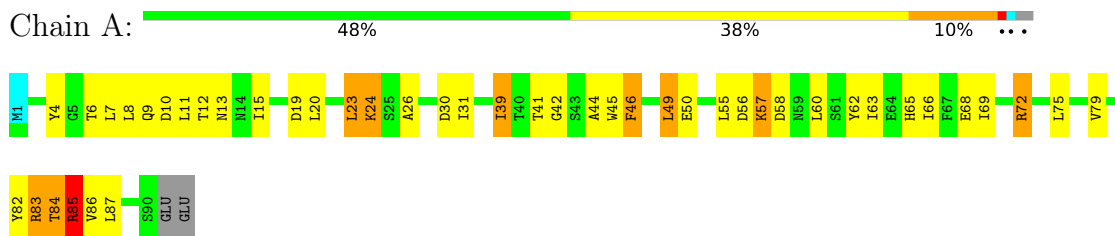
### 4.2.12 Score per residue for model 12

- Molecule 1: Astrocytic phosphoprotein PEA-15



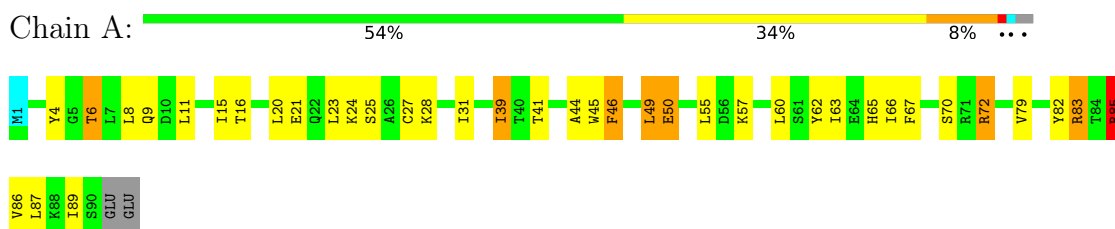
### 4.2.13 Score per residue for model 13

- Molecule 1: Astrocytic phosphoprotein PEA-15



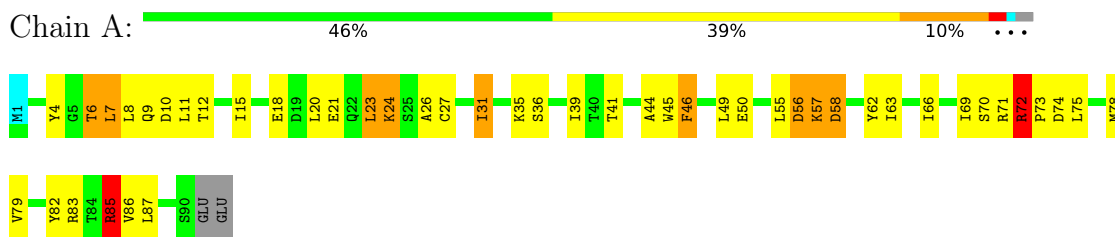
### 4.2.14 Score per residue for model 14

- Molecule 1: Astrocytic phosphoprotein PEA-15



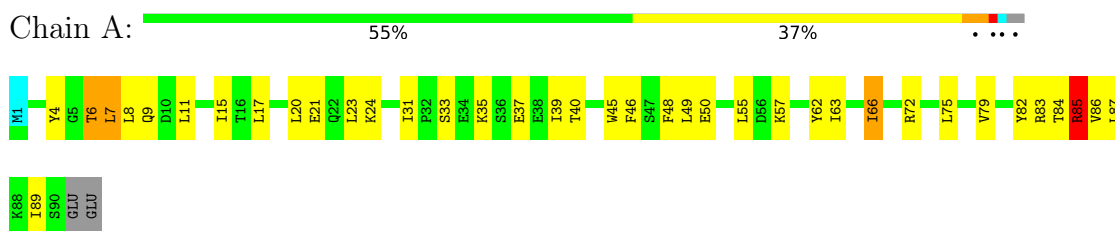
#### 4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: Astrocytic phosphoprotein PEA-15



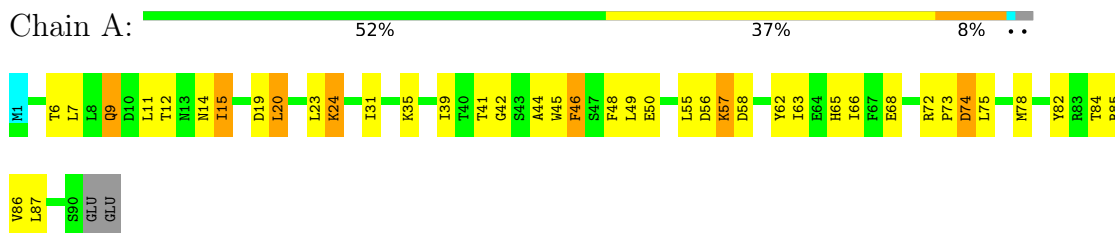
#### 4.2.16 Score per residue for model 16

- Molecule 1: Astrocytic phosphoprotein PEA-15



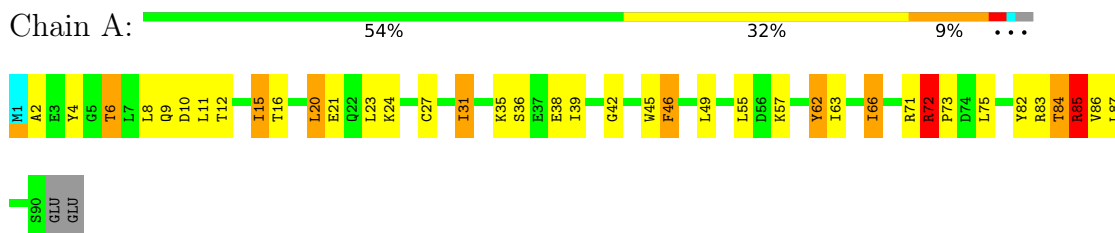
#### 4.2.17 Score per residue for model 17

- Molecule 1: Astrocytic phosphoprotein PEA-15



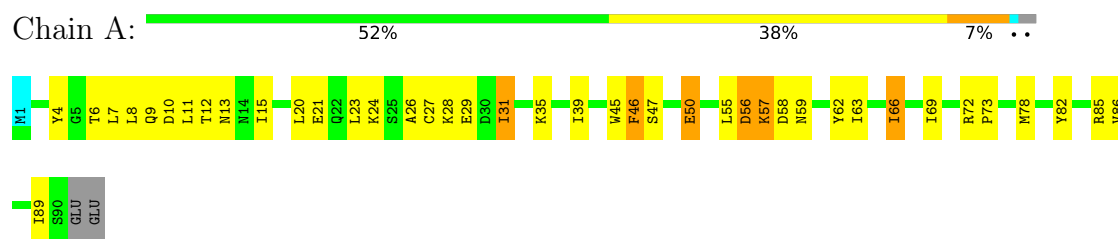
#### 4.2.18 Score per residue for model 18

- Molecule 1: Astrocytic phosphoprotein PEA-15



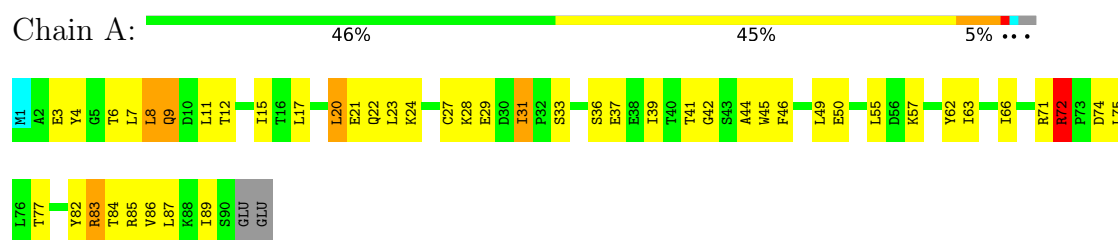
### 4.2.19 Score per residue for model 19

- Molecule 1: Astrocytic phosphoprotein PEA-15



### 4.2.20 Score per residue for model 20

- Molecule 1: Astrocytic phosphoprotein PEA-15



## 5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 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 |
|---------------|----------------|---------|
| X-PLOR NIH    | refinement     | 2.29    |

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                       | 1036           |
| Number of shifts mapped to atoms             | 1017           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 19             |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 82%            |

## 6 Model quality i

### 6.1 Standard geometry i

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     | 1.58±0.03    | 7±2/735 ( 0.9± 0.3%) | 1.47±0.03   | 2±1/993 ( 0.2± 0.1%) |
| All | All   | 1.58         | 136/14700 ( 0.9%)    | 1.47        | 46/19860 ( 0.2%)     |

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   | 1.5±1.3   |
| All | All   | 0         | 30        |

All unique bond 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(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|--------|-------------|----------|--------|-------|
|     |       |     |      |       |        |             |          | Worst  | Total |
| 1   | A     | 6   | THR  | C-O   | -10.06 | 1.12        | 1.24     | 15     | 20    |
| 1   | A     | 85  | ARG  | NE-CZ | 7.81   | 1.41        | 1.33     | 15     | 5     |
| 1   | A     | 52  | HIS  | C-N   | -7.76  | 1.24        | 1.33     | 1      | 1     |
| 1   | A     | 15  | ILE  | CA-CB | 7.11   | 1.62        | 1.54     | 15     | 9     |
| 1   | A     | 49  | LEU  | C-O   | -6.97  | 1.16        | 1.24     | 1      | 4     |
| 1   | A     | 50  | GLU  | N-CA  | 6.87   | 1.54        | 1.46     | 11     | 17    |
| 1   | A     | 62  | TYR  | C-N   | -6.68  | 1.25        | 1.33     | 18     | 3     |
| 1   | A     | 83  | ARG  | NE-CZ | 6.62   | 1.40        | 1.33     | 20     | 3     |
| 1   | A     | 20  | LEU  | CA-C  | -6.55  | 1.44        | 1.52     | 10     | 6     |
| 1   | A     | 16  | THR  | N-CA  | -6.42  | 1.37        | 1.45     | 14     | 5     |
| 1   | A     | 46  | PHE  | C-O   | -6.37  | 1.16        | 1.24     | 5      | 14    |
| 1   | A     | 58  | ASP  | CA-C  | -6.19  | 1.46        | 1.52     | 4      | 1     |
| 1   | A     | 56  | ASP  | CA-C  | -6.18  | 1.44        | 1.52     | 12     | 1     |
| 1   | A     | 59  | ASN  | C-N   | -6.14  | 1.24        | 1.33     | 9      | 2     |
| 1   | A     | 72  | ARG  | CA-C  | 6.06   | 1.60        | 1.52     | 10     | 1     |
| 1   | A     | 42  | GLY  | CA-C  | -5.92  | 1.45        | 1.52     | 6      | 1     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|-------|-------------|----------|--------|-------|
|     |       |     |      |       |       |             |          | Worst  | Total |
| 1   | A     | 66  | ILE  | CA-C  | -5.89 | 1.45        | 1.52     | 3      | 8     |
| 1   | A     | 58  | ASP  | C-N   | -5.75 | 1.25        | 1.33     | 4      | 1     |
| 1   | A     | 84  | THR  | CA-C  | 5.69  | 1.60        | 1.52     | 3      | 5     |
| 1   | A     | 40  | THR  | C-N   | -5.68 | 1.25        | 1.33     | 6      | 2     |
| 1   | A     | 76  | LEU  | N-CA  | 5.63  | 1.53        | 1.46     | 12     | 2     |
| 1   | A     | 8   | LEU  | C-N   | -5.63 | 1.26        | 1.34     | 11     | 4     |
| 1   | A     | 55  | LEU  | CA-CB | 5.59  | 1.60        | 1.52     | 9      | 1     |
| 1   | A     | 57  | LYS  | CA-C  | 5.44  | 1.59        | 1.52     | 5      | 2     |
| 1   | A     | 60  | LEU  | C-O   | -5.44 | 1.17        | 1.24     | 12     | 2     |
| 1   | A     | 84  | THR  | N-CA  | -5.39 | 1.40        | 1.46     | 20     | 2     |
| 1   | A     | 83  | ARG  | C-N   | -5.38 | 1.26        | 1.33     | 14     | 3     |
| 1   | A     | 72  | ARG  | C-N   | 5.37  | 1.40        | 1.34     | 2      | 2     |
| 1   | A     | 23  | LEU  | C-O   | -5.29 | 1.18        | 1.24     | 15     | 2     |
| 1   | A     | 31  | ILE  | CA-CB | 5.22  | 1.60        | 1.54     | 3      | 3     |
| 1   | A     | 77  | THR  | N-CA  | -5.14 | 1.40        | 1.46     | 4      | 1     |
| 1   | A     | 24  | LYS  | C-O   | -5.09 | 1.18        | 1.24     | 3      | 1     |
| 1   | A     | 81  | ASP  | C-O   | -5.02 | 1.18        | 1.24     | 7      | 1     |
| 1   | A     | 9   | GLN  | C-N   | -5.00 | 1.27        | 1.33     | 9      | 1     |

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     | 65  | HIS  | CA-CB-CG | 6.36  | 120.16      | 113.80   | 6      | 2     |
| 1   | A     | 56  | ASP  | N-CA-CB  | 6.33  | 118.86      | 110.25   | 19     | 1     |
| 1   | A     | 10  | ASP  | N-CA-CB  | 6.26  | 119.43      | 110.16   | 2      | 2     |
| 1   | A     | 9   | GLN  | N-CA-C   | 6.16  | 118.07      | 111.36   | 2      | 5     |
| 1   | A     | 10  | ASP  | N-CA-C   | 6.16  | 118.07      | 111.36   | 2      | 3     |
| 1   | A     | 72  | ARG  | CA-C-N   | 5.98  | 125.66      | 119.56   | 10     | 6     |
| 1   | A     | 72  | ARG  | C-N-CA   | 5.98  | 125.66      | 119.56   | 10     | 6     |
| 1   | A     | 49  | LEU  | N-CA-C   | -5.72 | 104.95      | 111.07   | 20     | 6     |
| 1   | A     | 56  | ASP  | CA-CB-CG | 5.45  | 118.05      | 112.60   | 6      | 2     |
| 1   | A     | 74  | ASP  | N-CA-C   | -5.43 | 105.28      | 111.14   | 9      | 2     |
| 1   | A     | 87  | LEU  | N-CA-C   | -5.31 | 105.50      | 111.28   | 8      | 3     |
| 1   | A     | 50  | GLU  | CB-CA-C  | -5.30 | 101.67      | 110.68   | 15     | 1     |
| 1   | A     | 71  | ARG  | CA-C-N   | 5.13  | 128.29      | 122.59   | 5      | 1     |
| 1   | A     | 71  | ARG  | C-N-CA   | 5.13  | 128.29      | 122.59   | 5      | 1     |
| 1   | A     | 58  | ASP  | CA-CB-CG | 5.06  | 117.66      | 112.60   | 15     | 1     |
| 1   | A     | 81  | ASP  | N-CA-CB  | 5.06  | 117.56      | 110.12   | 3      | 1     |
| 1   | A     | 30  | ASP  | CA-C-N   | -5.03 | 118.41      | 123.04   | 13     | 1     |
| 1   | A     | 30  | ASP  | C-N-CA   | -5.03 | 118.41      | 123.04   | 13     | 1     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|--------|------|-------------|----------|--------|-------|
|     |       |     |      |        |      |             |          | Worst  | Total |
| 1   | A     | 56  | ASP  | N-CA-C | 5.01 | 116.57      | 110.41   | 7      | 1     |

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     | 72  | ARG  | Sidechain | 9              |
| 1   | A     | 71  | ARG  | Sidechain | 7              |
| 1   | A     | 85  | ARG  | Sidechain | 7              |
| 1   | A     | 56  | ASP  | Mainchain | 4              |
| 1   | A     | 83  | ARG  | Sidechain | 3              |

## 6.2 Too-close contacts [i](#)

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     | 724   | 715      | 715      | 32±4    |
| All | All   | 14480 | 14300    | 14300    | 641     |

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 22.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:85:ARG:HH11 | 1:A:85:ARG:HB3  | 0.84     | 1.31        | 13     | 1     |
| 1:A:21:GLU:HA   | 1:A:24:LYS:HD3  | 0.81     | 1.51        | 20     | 3     |
| 1:A:55:LEU:HA   | 1:A:59:ASN:HD21 | 0.78     | 1.37        | 9      | 1     |
| 1:A:24:LYS:HE3  | 1:A:24:LYS:HA   | 0.78     | 1.55        | 13     | 4     |
| 1:A:9:GLN:HA    | 1:A:12:THR:HB   | 0.77     | 1.53        | 20     | 16    |
| 1:A:11:LEU:HD11 | 1:A:46:PHE:CZ   | 0.75     | 2.16        | 1      | 20    |
| 1:A:24:LYS:NZ   | 1:A:24:LYS:HA   | 0.74     | 1.96        | 5      | 3     |
| 1:A:20:LEU:HD23 | 1:A:23:LEU:HD12 | 0.73     | 1.60        | 2      | 11    |
| 1:A:78:MET:HA   | 1:A:78:MET:HE2  | 0.72     | 1.59        | 10     | 5     |
| 1:A:21:GLU:HG2  | 1:A:24:LYS:HE2  | 0.69     | 1.64        | 12     | 4     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:11:LEU:HD11 | 1:A:46:PHE:HZ   | 0.69     | 1.45        | 2      | 20    |
| 1:A:23:LEU:HD23 | 1:A:70:SER:HB3  | 0.69     | 1.63        | 7      | 3     |
| 1:A:21:GLU:HG2  | 1:A:24:LYS:HD3  | 0.68     | 1.65        | 16     | 1     |
| 1:A:55:LEU:HD12 | 1:A:63:ILE:HG21 | 0.67     | 1.66        | 8      | 19    |
| 1:A:20:LEU:HD11 | 1:A:42:GLY:HA2  | 0.67     | 1.65        | 3      | 7     |
| 1:A:57:LYS:HD2  | 1:A:58:ASP:N    | 0.67     | 2.03        | 4      | 7     |
| 1:A:28:LYS:HG3  | 1:A:29:GLU:HG3  | 0.67     | 1.66        | 8      | 4     |
| 1:A:24:LYS:HA   | 1:A:24:LYS:HZ2  | 0.67     | 1.49        | 8      | 3     |
| 1:A:20:LEU:HD12 | 1:A:23:LEU:HD12 | 0.65     | 1.69        | 16     | 7     |
| 1:A:24:LYS:HE3  | 1:A:45:TRP:CD1  | 0.63     | 2.29        | 1      | 3     |
| 1:A:82:TYR:CE1  | 1:A:86:VAL:HG21 | 0.63     | 2.29        | 15     | 20    |
| 1:A:49:LEU:HD11 | 1:A:62:TYR:HE2  | 0.62     | 1.54        | 16     | 7     |
| 1:A:33:SER:O    | 1:A:37:GLU:HG3  | 0.62     | 1.94        | 8      | 5     |
| 1:A:83:ARG:O    | 1:A:87:LEU:HG   | 0.62     | 1.95        | 15     | 3     |
| 1:A:57:LYS:HE3  | 1:A:58:ASP:HB2  | 0.61     | 1.71        | 11     | 1     |
| 1:A:27:CYS:SG   | 1:A:66:ILE:HD12 | 0.61     | 2.35        | 6      | 13    |
| 1:A:35:LYS:HA   | 1:A:35:LYS:HE2  | 0.61     | 1.71        | 8      | 1     |
| 1:A:17:LEU:O    | 1:A:21:GLU:HG2  | 0.60     | 1.95        | 11     | 2     |
| 1:A:72:ARG:HD2  | 1:A:75:LEU:HD13 | 0.60     | 1.71        | 16     | 3     |
| 1:A:7:LEU:HD22  | 1:A:82:TYR:CD2  | 0.60     | 2.31        | 20     | 5     |
| 1:A:85:ARG:HG2  | 1:A:85:ARG:HH11 | 0.60     | 1.56        | 15     | 3     |
| 1:A:62:TYR:O    | 1:A:66:ILE:HG12 | 0.58     | 1.98        | 4      | 20    |
| 1:A:33:SER:O    | 1:A:37:GLU:HG2  | 0.58     | 1.98        | 11     | 3     |
| 1:A:60:LEU:HD12 | 1:A:79:VAL:HG13 | 0.58     | 1.75        | 13     | 2     |
| 1:A:35:LYS:HG3  | 1:A:48:PHE:CE1  | 0.58     | 2.33        | 16     | 1     |
| 1:A:21:GLU:HA   | 1:A:24:LYS:HE2  | 0.58     | 1.75        | 18     | 4     |
| 1:A:21:GLU:HG2  | 1:A:24:LYS:CE   | 0.58     | 2.29        | 19     | 4     |
| 1:A:25:SER:HA   | 1:A:28:LYS:HE3  | 0.57     | 1.77        | 1      | 1     |
| 1:A:72:ARG:HG3  | 1:A:75:LEU:HD13 | 0.57     | 1.76        | 10     | 7     |
| 1:A:41:THR:HG23 | 1:A:44:ALA:HB2  | 0.57     | 1.75        | 12     | 10    |
| 1:A:57:LYS:HD3  | 1:A:57:LYS:N    | 0.57     | 2.15        | 5      | 5     |
| 1:A:39:ILE:HG21 | 1:A:45:TRP:HB2  | 0.56     | 1.77        | 15     | 6     |
| 1:A:26:ALA:HB1  | 1:A:69:ILE:HG13 | 0.56     | 1.76        | 11     | 2     |
| 1:A:39:ILE:HD13 | 1:A:45:TRP:HD1  | 0.56     | 1.60        | 8      | 3     |
| 1:A:4:TYR:O     | 1:A:8:LEU:HD13  | 0.55     | 2.02        | 20     | 15    |
| 1:A:83:ARG:O    | 1:A:87:LEU:HB2  | 0.55     | 2.02        | 7      | 11    |
| 1:A:7:LEU:HD13  | 1:A:82:TYR:HB2  | 0.55     | 1.79        | 3      | 5     |
| 1:A:7:LEU:HD22  | 1:A:82:TYR:CG   | 0.54     | 2.38        | 13     | 8     |
| 1:A:57:LYS:HD3  | 1:A:58:ASP:OD1  | 0.54     | 2.02        | 13     | 2     |
| 1:A:23:LEU:HD23 | 1:A:70:SER:CB   | 0.54     | 2.33        | 12     | 4     |
| 1:A:15:ILE:HG23 | 1:A:20:LEU:HB2  | 0.54     | 1.79        | 16     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:82:TYR:HA   | 1:A:85:ARG:HG3  | 0.54     | 1.78        | 2      | 2     |
| 1:A:24:LYS:HE3  | 1:A:36:SER:O    | 0.53     | 2.03        | 20     | 3     |
| 1:A:49:LEU:HD11 | 1:A:62:TYR:CE1  | 0.53     | 2.39        | 11     | 1     |
| 1:A:15:ILE:HG23 | 1:A:20:LEU:HG   | 0.53     | 1.80        | 6      | 8     |
| 1:A:49:LEU:HD11 | 1:A:62:TYR:CE2  | 0.53     | 2.39        | 5      | 8     |
| 1:A:84:THR:O    | 1:A:87:LEU:HB3  | 0.53     | 2.03        | 8      | 15    |
| 1:A:60:LEU:HD23 | 1:A:60:LEU:H    | 0.53     | 1.64        | 11     | 1     |
| 1:A:56:ASP:HB3  | 1:A:57:LYS:HD3  | 0.52     | 1.81        | 11     | 2     |
| 1:A:72:ARG:HD3  | 1:A:75:LEU:HD13 | 0.52     | 1.80        | 17     | 4     |
| 1:A:20:LEU:O    | 1:A:24:LYS:HG3  | 0.52     | 2.03        | 2      | 6     |
| 1:A:46:PHE:O    | 1:A:50:GLU:HG3  | 0.52     | 2.05        | 17     | 11    |
| 1:A:39:ILE:HD13 | 1:A:45:TRP:CD1  | 0.52     | 2.39        | 1      | 20    |
| 1:A:23:LEU:HD22 | 1:A:66:ILE:HG22 | 0.52     | 1.80        | 1      | 14    |
| 1:A:85:ARG:O    | 1:A:89:ILE:HG13 | 0.52     | 2.05        | 7      | 14    |
| 1:A:81:ASP:OD1  | 1:A:85:ARG:HD3  | 0.52     | 2.03        | 11     | 1     |
| 1:A:17:LEU:O    | 1:A:21:GLU:HG3  | 0.52     | 2.05        | 9      | 4     |
| 1:A:35:LYS:HG3  | 1:A:48:PHE:CZ   | 0.52     | 2.40        | 8      | 3     |
| 1:A:20:LEU:HD13 | 1:A:39:ILE:HG22 | 0.51     | 1.82        | 2      | 2     |
| 1:A:19:ASP:CG   | 1:A:72:ARG:HD2  | 0.51     | 2.30        | 17     | 1     |
| 1:A:55:LEU:HD12 | 1:A:63:ILE:CG2  | 0.51     | 2.36        | 20     | 14    |
| 1:A:6:THR:O     | 1:A:9:GLN:HB3   | 0.51     | 2.06        | 14     | 2     |
| 1:A:78:MET:HA   | 1:A:78:MET:CE   | 0.51     | 2.35        | 12     | 4     |
| 1:A:72:ARG:N    | 1:A:73:PRO:HD3  | 0.50     | 2.22        | 9      | 7     |
| 1:A:39:ILE:CG2  | 1:A:45:TRP:HB2  | 0.50     | 2.36        | 15     | 15    |
| 1:A:55:LEU:HD23 | 1:A:55:LEU:O    | 0.50     | 2.07        | 8      | 7     |
| 1:A:56:ASP:HB2  | 1:A:59:ASN:ND2  | 0.50     | 2.22        | 19     | 1     |
| 1:A:24:LYS:HB3  | 1:A:36:SER:OG   | 0.49     | 2.07        | 3      | 2     |
| 1:A:36:SER:HA   | 1:A:39:ILE:HD12 | 0.49     | 1.84        | 20     | 4     |
| 1:A:82:TYR:HA   | 1:A:85:ARG:HG2  | 0.49     | 1.82        | 7      | 8     |
| 1:A:3:GLU:H     | 1:A:3:GLU:CD    | 0.49     | 2.16        | 20     | 2     |
| 1:A:62:TYR:C    | 1:A:62:TYR:CD1  | 0.47     | 2.92        | 18     | 1     |
| 1:A:24:LYS:HD3  | 1:A:39:ILE:HB   | 0.47     | 1.87        | 11     | 2     |
| 1:A:10:ASP:HA   | 1:A:13:ASN:ND2  | 0.47     | 2.25        | 13     | 2     |
| 1:A:57:LYS:HD2  | 1:A:57:LYS:C    | 0.47     | 2.34        | 7      | 4     |
| 1:A:24:LYS:HE3  | 1:A:45:TRP:CG   | 0.47     | 2.45        | 8      | 1     |
| 1:A:19:ASP:OD1  | 1:A:72:ARG:HD3  | 0.47     | 2.09        | 13     | 1     |
| 1:A:60:LEU:HD12 | 1:A:79:VAL:HG12 | 0.47     | 1.86        | 9      | 2     |
| 1:A:21:GLU:HA   | 1:A:24:LYS:HE3  | 0.46     | 1.86        | 2      | 1     |
| 1:A:35:LYS:O    | 1:A:39:ILE:HG13 | 0.46     | 2.10        | 6      | 7     |
| 1:A:72:ARG:CG   | 1:A:75:LEU:HD13 | 0.46     | 2.40        | 20     | 2     |
| 1:A:27:CYS:HB3  | 1:A:31:ILE:HG22 | 0.46     | 1.85        | 15     | 3     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:57:LYS:HG2  | 1:A:58:ASP:OD1  | 0.46     | 2.10        | 5      | 2     |
| 1:A:56:ASP:H    | 1:A:59:ASN:HD21 | 0.46     | 1.52        | 4      | 1     |
| 1:A:74:ASP:O    | 1:A:78:MET:HG3  | 0.46     | 2.10        | 9      | 1     |
| 1:A:4:TYR:HB2   | 1:A:82:TYR:OH   | 0.45     | 2.10        | 4      | 3     |
| 1:A:19:ASP:OD2  | 1:A:72:ARG:HD2  | 0.45     | 2.11        | 7      | 2     |
| 1:A:39:ILE:HG23 | 1:A:45:TRP:HB2  | 0.45     | 1.89        | 4      | 1     |
| 1:A:41:THR:CG2  | 1:A:44:ALA:HB2  | 0.45     | 2.41        | 13     | 6     |
| 1:A:24:LYS:O    | 1:A:28:LYS:HG3  | 0.45     | 2.11        | 3      | 1     |
| 1:A:45:TRP:O    | 1:A:49:LEU:HB2  | 0.45     | 2.12        | 15     | 2     |
| 1:A:7:LEU:HD21  | 1:A:79:VAL:HA   | 0.45     | 1.89        | 15     | 2     |
| 1:A:8:LEU:HG    | 1:A:46:PHE:CD1  | 0.45     | 2.45        | 20     | 1     |
| 1:A:56:ASP:H    | 1:A:59:ASN:ND2  | 0.45     | 2.10        | 12     | 2     |
| 1:A:25:SER:HA   | 1:A:28:LYS:NZ   | 0.45     | 2.26        | 14     | 1     |
| 1:A:35:LYS:HD3  | 1:A:38:GLU:CD   | 0.44     | 2.37        | 18     | 1     |
| 1:A:26:ALA:HB1  | 1:A:69:ILE:CD1  | 0.44     | 2.43        | 6      | 5     |
| 1:A:22:GLN:NE2  | 1:A:71:ARG:H    | 0.44     | 2.10        | 2      | 3     |
| 1:A:15:ILE:CG2  | 1:A:20:LEU:HG   | 0.44     | 2.42        | 6      | 3     |
| 1:A:85:ARG:HG3  | 1:A:86:VAL:HG23 | 0.44     | 1.89        | 7      | 1     |
| 1:A:15:ILE:HD12 | 1:A:20:LEU:HG   | 0.44     | 1.89        | 4      | 1     |
| 1:A:21:GLU:CD   | 1:A:24:LYS:HZ3  | 0.44     | 2.19        | 11     | 1     |
| 1:A:39:ILE:HG22 | 1:A:39:ILE:O    | 0.44     | 2.13        | 13     | 4     |
| 1:A:28:LYS:HG3  | 1:A:29:GLU:N    | 0.44     | 2.28        | 11     | 1     |
| 1:A:20:LEU:O    | 1:A:24:LYS:HG2  | 0.43     | 2.13        | 5      | 3     |
| 1:A:65:HIS:O    | 1:A:68:GLU:HB3  | 0.43     | 2.14        | 17     | 4     |
| 1:A:20:LEU:HD21 | 1:A:39:ILE:HG22 | 0.43     | 1.90        | 12     | 3     |
| 1:A:31:ILE:HB   | 1:A:62:TYR:OH   | 0.43     | 2.13        | 18     | 1     |
| 1:A:6:THR:O     | 1:A:10:ASP:N    | 0.43     | 2.51        | 15     | 7     |
| 1:A:85:ARG:C    | 1:A:85:ARG:HD3  | 0.43     | 2.39        | 5      | 1     |
| 1:A:27:CYS:O    | 1:A:31:ILE:HG22 | 0.43     | 2.13        | 8      | 2     |
| 1:A:22:GLN:HG3  | 1:A:70:SER:OG   | 0.43     | 2.13        | 9      | 1     |
| 1:A:65:HIS:O    | 1:A:69:ILE:HG12 | 0.42     | 2.14        | 6      | 1     |
| 1:A:62:TYR:CD1  | 1:A:62:TYR:C    | 0.42     | 2.97        | 7      | 2     |
| 1:A:10:ASP:HB3  | 1:A:78:MET:CE   | 0.42     | 2.44        | 19     | 1     |
| 1:A:4:TYR:O     | 1:A:7:LEU:HB3   | 0.42     | 2.14        | 1      | 4     |
| 1:A:11:LEU:HD11 | 1:A:46:PHE:CE2  | 0.42     | 2.50        | 7      | 8     |
| 1:A:56:ASP:HB2  | 1:A:59:ASN:HD21 | 0.42     | 1.73        | 19     | 1     |
| 1:A:7:LEU:HG    | 1:A:82:TYR:CG   | 0.42     | 2.50        | 9      | 1     |
| 1:A:47:SER:HA   | 1:A:50:GLU:OE1  | 0.41     | 2.15        | 5      | 2     |
| 1:A:18:GLU:O    | 1:A:21:GLU:HB2  | 0.41     | 2.14        | 15     | 1     |
| 1:A:24:LYS:HE3  | 1:A:24:LYS:CA   | 0.41     | 2.39        | 15     | 1     |
| 1:A:74:ASP:O    | 1:A:77:THR:HB   | 0.41     | 2.15        | 20     | 1     |

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| Atom-1         | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|----------------|-----------------|----------|-------------|--------|-------|
|                |                 |          |             | Worst  | Total |
| 1:A:74:ASP:O   | 1:A:78:MET:HG2  | 0.41     | 2.14        | 15     | 1     |
| 1:A:4:TYR:CZ   | 1:A:8:LEU:HD11  | 0.41     | 2.51        | 2      | 1     |
| 1:A:21:GLU:CG  | 1:A:24:LYS:HE2  | 0.41     | 2.40        | 12     | 1     |
| 1:A:19:ASP:OD1 | 1:A:72:ARG:HD2  | 0.41     | 2.16        | 5      | 1     |
| 1:A:35:LYS:HA  | 1:A:38:GLU:HG2  | 0.41     | 1.93        | 18     | 1     |
| 1:A:60:LEU:O   | 1:A:63:ILE:HG12 | 0.41     | 2.16        | 8      | 2     |
| 1:A:24:LYS:HA  | 1:A:24:LYS:CE   | 0.41     | 2.39        | 13     | 1     |
| 1:A:83:ARG:HD3 | 1:A:83:ARG:C    | 0.41     | 2.40        | 16     | 2     |
| 1:A:56:ASP:C   | 1:A:58:ASP:H    | 0.41     | 2.24        | 12     | 1     |
| 1:A:14:ASN:ND2 | 1:A:78:MET:HE1  | 0.41     | 2.31        | 17     | 1     |
| 1:A:12:THR:HA  | 1:A:15:ILE:HB   | 0.40     | 1.92        | 19     | 1     |
| 1:A:57:LYS:HD3 | 1:A:57:LYS:H    | 0.40     | 1.73        | 5      | 1     |
| 1:A:10:ASP:HB3 | 1:A:78:MET:HE1  | 0.40     | 1.92        | 19     | 1     |
| 1:A:39:ILE:O   | 1:A:39:ILE:HG22 | 0.40     | 2.17        | 1      | 1     |
| 1:A:67:PHE:CD2 | 1:A:79:VAL:HG21 | 0.40     | 2.52        | 14     | 1     |
| 1:A:55:LEU:HA  | 1:A:59:ASN:OD1  | 0.40     | 2.16        | 4      | 1     |
| 1:A:57:LYS:HD2 | 1:A:58:ASP:HB2  | 0.40     | 1.94        | 7      | 1     |
| 1:A:21:GLU:HG2 | 1:A:24:LYS:CD   | 0.40     | 2.44        | 16     | 1     |

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

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     | 88/92 (96%)     | 83±1 (94±1%) | 5±1 (6±1%) | 0±0 (0±0%) | 44 80       |
| All | All   | 1760/1840 (96%) | 1654 (94%)   | 103 (6%)   | 3 (0%)     | 44 80       |

All 1 unique Ramachandran outliers are listed below.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 39  | ILE  | 3              |

### 6.3.2 Protein sidechains [i](#)

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     | 84/87 (97%)     | 80±2 (95±3%) | 4±1 (5±2%) | 25 76       |
| All | All   | 1668/1740 (96%) | 1591 (95%)   | 77 (5%)    | 25 76       |

All 14 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  | ILE  | 20             |
| 1   | A     | 57  | LYS  | 20             |
| 1   | A     | 24  | LYS  | 8              |
| 1   | A     | 85  | ARG  | 6              |
| 1   | A     | 7   | LEU  | 5              |
| 1   | A     | 78  | MET  | 5              |
| 1   | A     | 87  | LEU  | 5              |
| 1   | A     | 3   | GLU  | 2              |
| 1   | A     | 55  | LEU  | 1              |
| 1   | A     | 83  | ARG  | 1              |
| 1   | A     | 88  | LYS  | 1              |
| 1   | A     | 59  | ASN  | 1              |
| 1   | A     | 15  | ILE  | 1              |
| 1   | A     | 74  | ASP  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation i

The completeness of assignment taking into account all chemical shift lists is 82% for the well-defined parts and 81% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping i

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                  | 1036 |
| Number of shifts mapped to atoms        | 1017 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 19   |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 4    |

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 19 occurrences are reported below.

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 91  | GLU  | H    | 8.423      | .           | 1         |
| 1       | A     | 91  | GLU  | HA   | 4.235      | .           | 1         |
| 1       | A     | 91  | GLU  | HB2  | 2.04       | .           | .         |
| 1       | A     | 91  | GLU  | HB3  | 1.956      | .           | .         |
| 1       | A     | 91  | GLU  | HG2  | 2.189      | .           | .         |
| 1       | A     | 91  | GLU  | HG3  | 2.263      | .           | .         |
| 1       | A     | 91  | GLU  | CA   | 57.275     | .           | 1         |
| 1       | A     | 91  | GLU  | CB   | 30.253     | .           | 1         |
| 1       | A     | 91  | GLU  | CG   | 36.519     | .           | 1         |
| 1       | A     | 91  | GLU  | N    | 122.841    | .           | 1         |
| 1       | A     | 92  | GLU  | H    | 8.304      | .           | 1         |
| 1       | A     | 92  | GLU  | HA   | 4.171      | .           | 1         |
| 1       | A     | 92  | GLU  | HB2  | 1.993      | .           | .         |
| 1       | A     | 92  | GLU  | HB3  | 1.91       | .           | .         |

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| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 92  | GLU  | HG2  | 2.227      | .           | .         |
| 1       | A     | 92  | GLU  | CA   | 57.205     | .           | 1         |
| 1       | A     | 92  | GLU  | CB   | 30.256     | .           | 1         |
| 1       | A     | 92  | GLU  | CG   | 36.517     | .           | 1         |
| 1       | A     | 92  | GLU  | N    | 120.39     | .           | 1         |

### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 92       | $-0.49 \pm 0.40$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 90       | $0.48 \pm 0.12$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 0        | —                               | None (insufficient data)   |
| $^{15}\text{N}$        | 89       | $0.74 \pm 0.20$                 | Should be applied          |

### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 82%, i.e. 1009 atoms were assigned a chemical shift out of a possible 1238. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | $^1\text{H}$   | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 354/443 (80%)   | 178/178 (100%) | 89/178 (50%)    | 87/87 (100%)    |
| Sidechain | 583/712 (82%)   | 381/460 (83%)  | 193/228 (85%)   | 9/24 (38%)      |
| Aromatic  | 72/83 (87%)     | 36/41 (88%)    | 35/39 (90%)     | 1/3 (33%)       |
| Overall   | 1009/1238 (82%) | 595/679 (88%)  | 317/445 (71%)   | 97/114 (85%)    |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 81%, i.e. 1017 atoms were assigned a chemical shift out of a possible 1253. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|-----------------|---------------|-----------------|-----------------|
| Backbone  | 356/448 (79%)   | 179/180 (99%) | 90/180 (50%)    | 87/88 (99%)     |
| Sidechain | 589/722 (82%)   | 385/467 (82%) | 195/231 (84%)   | 9/24 (38%)      |
| Aromatic  | 72/83 (87%)     | 36/41 (88%)   | 35/39 (90%)     | 1/3 (33%)       |
| Overall   | 1017/1253 (81%) | 600/688 (87%) | 320/450 (71%)   | 97/115 (84%)    |

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

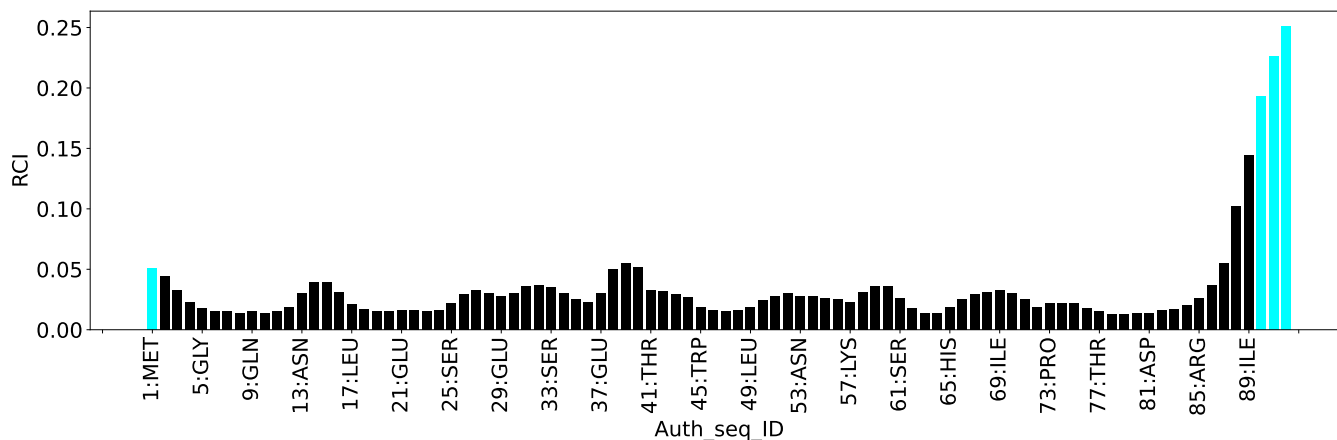
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 85  | ARG  | NE   | 113.25     | 76.53 – 92.65       | 17.8    |
| 1       | A     | 83  | ARG  | NE   | 112.94     | 76.53 – 92.65       | 17.6    |
| 1       | A     | 72  | ARG  | NE   | 110.70     | 76.53 – 92.65       | 16.2    |
| 1       | A     | 24  | LYS  | CE   | 34.76      | 37.57 – 46.21       | -8.2    |

### 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                                | 1993  |
| Intra-residue ( $ i-j =0$ )                              | 341   |
| Sequential ( $ i-j =1$ )                                 | 469   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 614   |
| Long range ( $ i-j \geq 5$ )                             | 483   |
| Inter-chain  | 0     |
| Hydrogen bond restraints                                 | 86    |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 232   |
| Number of unmapped restraints                            | 9     |
| Number of restraints per residue                         | 24.2  |
| Number of long range restraints per residue <sup>1</sup> | 5.2   |

<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)  | 65.8                                   | 0.2     |
| 0.2-0.5 (Medium) | 14.6                                   | 0.39    |
| >0.5 (Large)     | None                                   | None    |

### 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)   | 1.1                                    | 4.42    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis

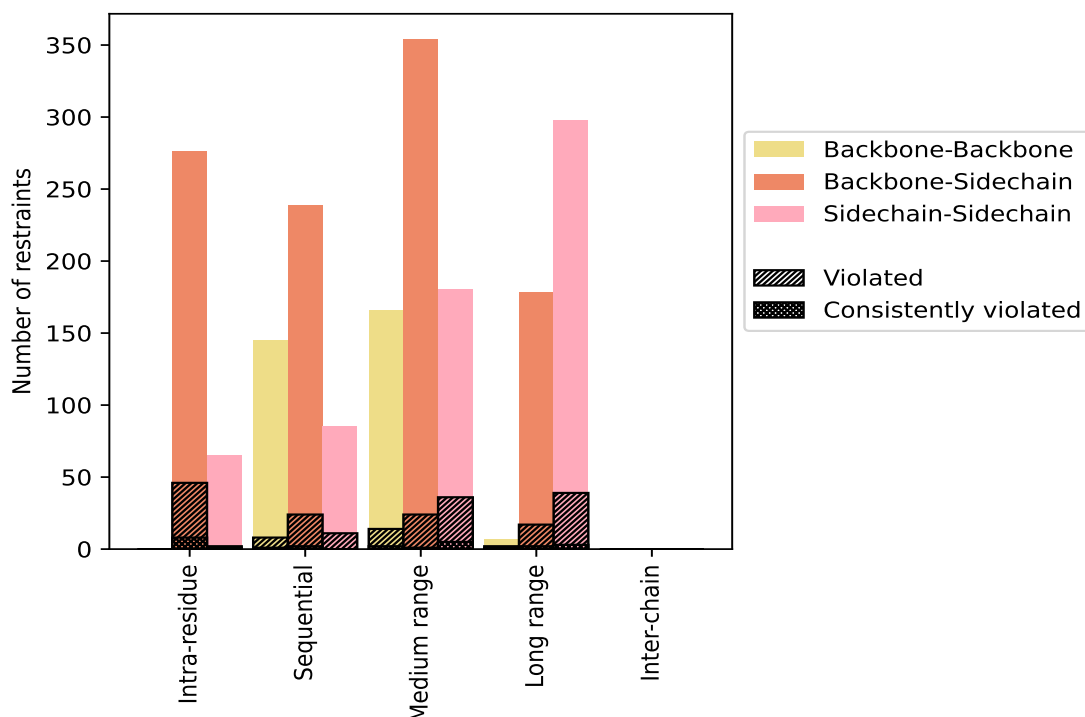
### 9.1 Summary of distance violations

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> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>341</b>  | <b>17.1</b>    | <b>48</b>             | <b>14.1</b>    | <b>2.4</b>     | <b>9</b>                           | <b>2.6</b>     | <b>0.5</b>     |
| Backbone-Backbone   | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 276         | 13.8           | 46                    | 16.7           | 2.3            | 8                                  | 2.9            | 0.4            |
| Sidechain-Sidechain   | 65          | 3.3            | 2                     | 3.1            | 0.1            | 1                                  | 1.5            | 0.1            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>469</b>  | <b>23.5</b>    | <b>43</b>             | <b>9.2</b>     | <b>2.2</b>     | <b>3</b>                           | <b>0.6</b>     | <b>0.2</b>     |
| Backbone-Backbone   | 145         | 7.3            | 8                     | 5.5            | 0.4            | 1                                  | 0.7            | 0.1            |
| Backbone-Sidechain  | 239         | 12.0           | 24                    | 10.0           | 1.2            | 2                                  | 0.8            | 0.1            |
| Sidechain-Sidechain   | 85          | 4.3            | 11                    | 12.9           | 0.6            | 0                                  | 0.0            | 0.0            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>614</b>  | <b>30.8</b>    | <b>73</b>             | <b>11.9</b>    | <b>3.7</b>     | <b>8</b>                           | <b>1.3</b>     | <b>0.4</b>     |
| Backbone-Backbone   | 166         | 8.3            | 14                    | 8.4            | 0.7            | 2                                  | 1.2            | 0.1            |
| Backbone-Sidechain  | 268         | 13.4           | 23                    | 8.6            | 1.2            | 1                                  | 0.4            | 0.1            |
| Sidechain-Sidechain   | 180         | 9.0            | 36                    | 20.0           | 1.8            | 5                                  | 2.8            | 0.3            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>483</b>  | <b>24.2</b>    | <b>58</b>             | <b>12.0</b>    | <b>2.9</b>     | <b>6</b>                           | <b>1.2</b>     | <b>0.3</b>     |
| Backbone-Backbone   | 7           | 0.4            | 2                     | 28.6           | 0.1            | 1                                  | 14.3           | 0.1            |
| Backbone-Sidechain  | 178         | 8.9            | 17                    | 9.6            | 0.9            | 2                                  | 1.1            | 0.1            |
| Sidechain-Sidechain   | 298         | 15.0           | 39                    | 13.1           | 2.0            | 3                                  | 1.0            | 0.2            |
| <b>Inter-chain</b>  | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| 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            |
| <b>Hydrogen bond</b>  | <b>86</b>   | <b>4.3</b>     | <b>1</b>              | <b>1.2</b>     | <b>0.1</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>   | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>  | <b>1993</b> | <b>100.0</b>   | <b>223</b>            | <b>11.2</b>    | <b>11.2</b>    | <b>26</b>                          | <b>1.3</b>     | <b>1.3</b>     |
| Backbone-Backbone   | 318         | 16.0           | 24                    | 7.5            | 1.2            | 4                                  | 1.3            | 0.2            |
| Backbone-Sidechain  | 1047        | 52.5           | 111                   | 10.6           | 5.6            | 13                                 | 1.2            | 0.7            |
| Sidechain-Sidechain   | 628         | 31.5           | 88                    | 14.0           | 4.4            | 9                                  | 1.4            | 0.5            |

<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 disulfid 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        | 21                   | 18              | 30              | 18              | 0               | 87    | 0.16     | 0.33    | 0.06                | 0.15       |
| 2        | 20                   | 17              | 28              | 22              | 0               | 87    | 0.16     | 0.31    | 0.05                | 0.15       |
| 3        | 20                   | 20              | 26              | 17              | 0               | 83    | 0.16     | 0.34    | 0.05                | 0.15       |
| 4        | 21                   | 22              | 27              | 17              | 0               | 87    | 0.16     | 0.36    | 0.05                | 0.14       |
| 5        | 21                   | 18              | 25              | 19              | 0               | 83    | 0.16     | 0.32    | 0.05                | 0.15       |
| 6        | 17                   | 14              | 29              | 20              | 0               | 80    | 0.16     | 0.3     | 0.05                | 0.16       |
| 7        | 19                   | 19              | 29              | 18              | 0               | 85    | 0.16     | 0.38    | 0.05                | 0.15       |
| 8        | 20                   | 22              | 31              | 18              | 0               | 91    | 0.16     | 0.37    | 0.06                | 0.14       |
| 9        | 18                   | 15              | 32              | 20              | 0               | 85    | 0.16     | 0.32    | 0.06                | 0.15       |
| 10       | 24                   | 20              | 26              | 22              | 0               | 92    | 0.16     | 0.36    | 0.06                | 0.15       |

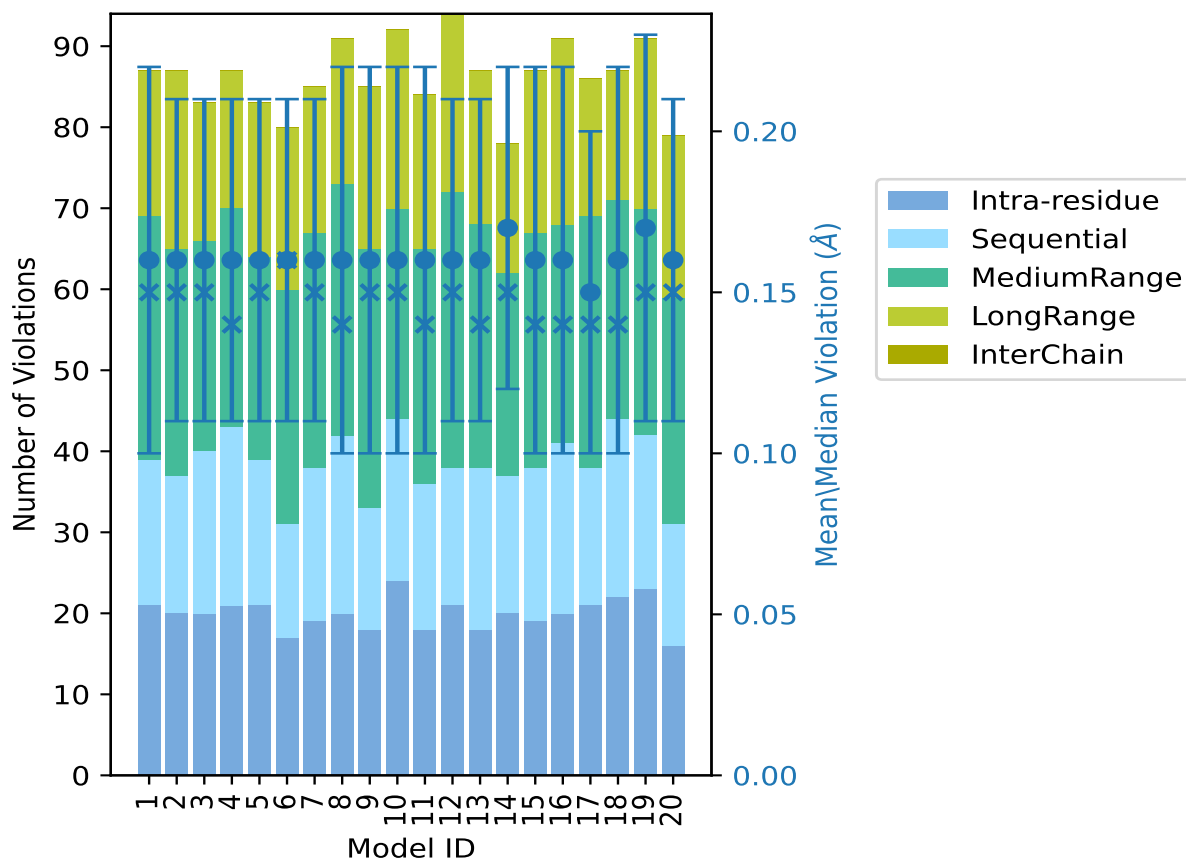
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 18                   | 18              | 29              | 19              | 0               | 84    | 0.16     | 0.34    | 0.06                | 0.14       |
| 12       | 21                   | 17              | 34              | 22              | 0               | 94    | 0.16     | 0.38    | 0.05                | 0.15       |
| 13       | 18                   | 20              | 30              | 19              | 0               | 87    | 0.16     | 0.39    | 0.05                | 0.14       |
| 14       | 20                   | 17              | 25              | 16              | 0               | 78    | 0.17     | 0.32    | 0.05                | 0.15       |
| 15       | 19                   | 19              | 29              | 20              | 0               | 87    | 0.16     | 0.35    | 0.06                | 0.14       |
| 16       | 20                   | 21              | 27              | 23              | 0               | 91    | 0.16     | 0.39    | 0.06                | 0.14       |
| 17       | 21                   | 17              | 31              | 17              | 0               | 86    | 0.15     | 0.37    | 0.05                | 0.14       |
| 18       | 22                   | 22              | 27              | 16              | 0               | 87    | 0.16     | 0.33    | 0.06                | 0.14       |
| 19       | 23                   | 19              | 28              | 21              | 0               | 91    | 0.17     | 0.32    | 0.06                | 0.15       |
| 20       | 16                   | 15              | 28              | 20              | 0               | 79    | 0.16     | 0.36    | 0.05                | 0.15       |

<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



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

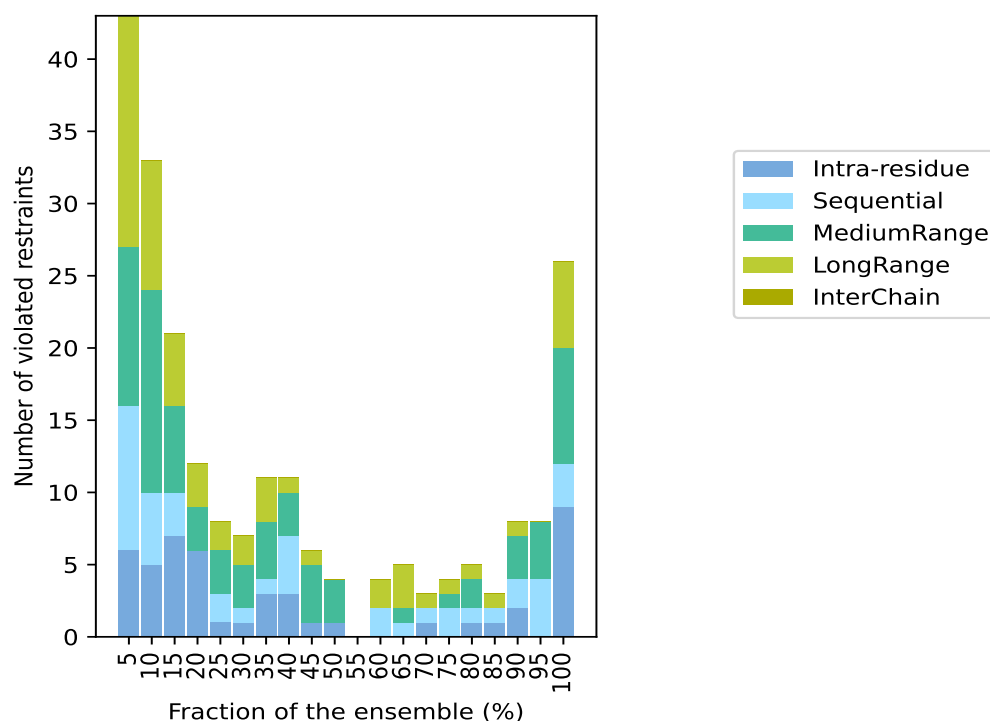
### 9.3 Distance violation statistics for the ensemble

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, 1685(IR:293, SQ:426, MR:541, LR:425, 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>       | %     |
| 6                             | 10              | 11              | 16              | 0               | 43    | 1                        | 5.0   |
| 5                             | 5               | 14              | 9               | 0               | 33    | 2                        | 10.0  |
| 7                             | 3               | 6               | 5               | 0               | 21    | 3                        | 15.0  |
| 6                             | 0               | 3               | 3               | 0               | 12    | 4                        | 20.0  |
| 1                             | 2               | 3               | 2               | 0               | 8     | 5                        | 25.0  |
| 1                             | 1               | 3               | 2               | 0               | 7     | 6                        | 30.0  |
| 3                             | 1               | 4               | 3               | 0               | 11    | 7                        | 35.0  |
| 3                             | 4               | 3               | 1               | 0               | 11    | 8                        | 40.0  |
| 1                             | 0               | 4               | 1               | 0               | 6     | 9                        | 45.0  |
| 1                             | 0               | 3               | 0               | 0               | 4     | 10                       | 50.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 11                       | 55.0  |
| 0                             | 2               | 0               | 2               | 0               | 4     | 12                       | 60.0  |
| 0                             | 1               | 1               | 3               | 0               | 5     | 13                       | 65.0  |
| 1                             | 1               | 0               | 1               | 0               | 3     | 14                       | 70.0  |
| 0                             | 2               | 1               | 1               | 0               | 4     | 15                       | 75.0  |
| 1                             | 1               | 2               | 1               | 0               | 5     | 16                       | 80.0  |
| 1                             | 1               | 0               | 1               | 0               | 3     | 17                       | 85.0  |
| 2                             | 2               | 3               | 1               | 0               | 8     | 18                       | 90.0  |
| 0                             | 4               | 4               | 0               | 0               | 8     | 19                       | 95.0  |
| 9                             | 3               | 8               | 6               | 0               | 26    | 20                       | 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

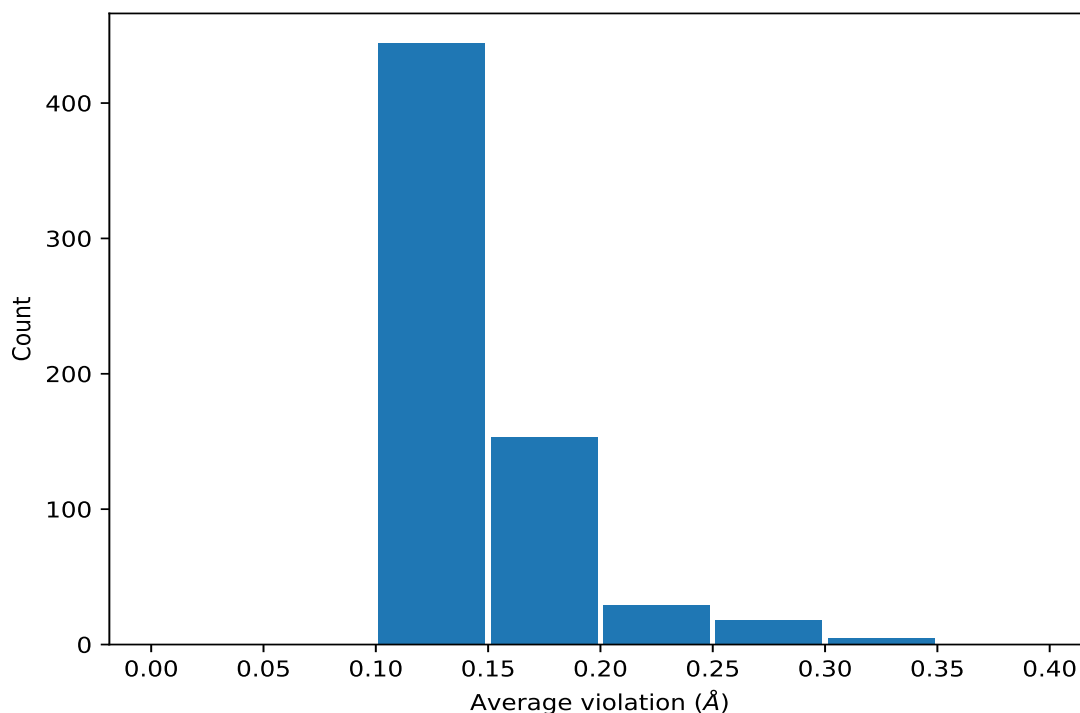
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1462) | 1:66:A:ILE:HG12 | 1:67:A:PHE:H    | 20                  | 0.33     | 0.04                | 0.32       |
| (1,1462) | 1:66:A:ILE:HG13 | 1:67:A:PHE:H    | 20                  | 0.33     | 0.04                | 0.32       |
| (1,631)  | 1:25:A:SER:H    | 1:27:A:CYS:H    | 20                  | 0.28     | 0.03                | 0.29       |
| (1,1673) | 1:77:A:THR:HG21 | 1:77:A:THR:H    | 20                  | 0.28     | 0.01                | 0.28       |
| (1,1673) | 1:77:A:THR:HG22 | 1:77:A:THR:H    | 20                  | 0.28     | 0.01                | 0.28       |
| (1,1673) | 1:77:A:THR:HG23 | 1:77:A:THR:H    | 20                  | 0.28     | 0.01                | 0.28       |
| (1,1806) | 1:84:A:THR:HG21 | 1:84:A:THR:H    | 20                  | 0.27     | 0.03                | 0.28       |
| (1,1806) | 1:84:A:THR:HG22 | 1:84:A:THR:H    | 20                  | 0.27     | 0.03                | 0.28       |
| (1,1806) | 1:84:A:THR:HG23 | 1:84:A:THR:H    | 20                  | 0.27     | 0.03                | 0.28       |
| (1,314)  | 1:12:A:THR:HG21 | 1:12:A:THR:H    | 20                  | 0.25     | 0.01                | 0.25       |
| (1,314)  | 1:12:A:THR:HG22 | 1:12:A:THR:H    | 20                  | 0.25     | 0.01                | 0.25       |
| (1,314)  | 1:12:A:THR:HG23 | 1:12:A:THR:H    | 20                  | 0.25     | 0.01                | 0.25       |
| (1,894)  | 1:39:A:ILE:HD11 | 1:45:A:TRP:HH2  | 20                  | 0.25     | 0.06                | 0.25       |
| (1,894)  | 1:39:A:ILE:HD12 | 1:45:A:TRP:HH2  | 20                  | 0.25     | 0.06                | 0.25       |
| (1,894)  | 1:39:A:ILE:HD13 | 1:45:A:TRP:HH2  | 20                  | 0.25     | 0.06                | 0.25       |
| (1,570)  | 1:22:A:GLN:H    | 1:66:A:ILE:HG21 | 20                  | 0.2      | 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) |
|----------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,570)  | 1:22:A:GLN:H   | 1:66:A:ILE:HG22 | 20                  | 0.2      | 0.04                | 0.2        |
| (1,570)  | 1:22:A:GLN:H   | 1:66:A:ILE:HG23 | 20                  | 0.2      | 0.04                | 0.2        |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD11 | 20                  | 0.2      | 0.01                | 0.2        |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD12 | 20                  | 0.2      | 0.01                | 0.2        |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD13 | 20                  | 0.2      | 0.01                | 0.2        |
| (1,1105) | 1:49:A:LEU:HB2 | 1:52:A:HIS:HD2  | 20                  | 0.2      | 0.04                | 0.2        |
| (1,1105) | 1:49:A:LEU:HB3 | 1:52:A:HIS:HD2  | 20                  | 0.2      | 0.04                | 0.2        |
| (1,341)  | 1:12:A:THR:H   | 1:46:A:PHE:HE1  | 20                  | 0.19     | 0.02                | 0.2        |
| (1,341)  | 1:12:A:THR:H   | 1:46:A:PHE:HE2  | 20                  | 0.19     | 0.02                | 0.2        |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG12 | 20                  | 0.19     | 0.02                | 0.19       |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG13 | 20                  | 0.19     | 0.02                | 0.19       |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG12 | 20                  | 0.19     | 0.02                | 0.19       |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG13 | 20                  | 0.19     | 0.02                | 0.19       |
| (1,112)  | 1:6:A:THR:HG21 | 1:6:A:THR:H     | 20                  | 0.19     | 0.01                | 0.19       |
| (1,112)  | 1:6:A:THR:HG22 | 1:6:A:THR:H     | 20                  | 0.19     | 0.01                | 0.19       |
| (1,112)  | 1:6:A:THR:HG23 | 1:6:A:THR:H     | 20                  | 0.19     | 0.01                | 0.19       |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD11 | 20                  | 0.19     | 0.01                | 0.18       |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD12 | 20                  | 0.19     | 0.01                | 0.18       |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD13 | 20                  | 0.19     | 0.01                | 0.18       |
| (1,67)   | 1:4:A:TYR:HB2  | 1:7:A:LEU:HD11  | 20                  | 0.18     | 0.07                | 0.14       |
| (1,67)   | 1:4:A:TYR:HB2  | 1:7:A:LEU:HD12  | 20                  | 0.18     | 0.07                | 0.14       |
| (1,67)   | 1:4:A:TYR:HB2  | 1:7:A:LEU:HD13  | 20                  | 0.18     | 0.07                | 0.14       |
| (1,67)   | 1:4:A:TYR:HB2  | 1:7:A:LEU:HD21  | 20                  | 0.18     | 0.07                | 0.14       |
| (1,67)   | 1:4:A:TYR:HB2  | 1:7:A:LEU:HD22  | 20                  | 0.18     | 0.07                | 0.14       |
| (1,67)   | 1:4:A:TYR:HB2  | 1:7:A:LEU:HD23  | 20                  | 0.18     | 0.07                | 0.14       |
| (1,67)   | 1:4:A:TYR:HB3  | 1:7:A:LEU:HD11  | 20                  | 0.18     | 0.07                | 0.14       |
| (1,67)   | 1:4:A:TYR:HB3  | 1:7:A:LEU:HD12  | 20                  | 0.18     | 0.07                | 0.14       |
| (1,67)   | 1:4:A:TYR:HB3  | 1:7:A:LEU:HD13  | 20                  | 0.18     | 0.07                | 0.14       |
| (1,67)   | 1:4:A:TYR:HB3  | 1:7:A:LEU:HD21  | 20                  | 0.18     | 0.07                | 0.14       |
| (1,67)   | 1:4:A:TYR:HB3  | 1:7:A:LEU:HD22  | 20                  | 0.18     | 0.07                | 0.14       |
| (1,67)   | 1:4:A:TYR:HB3  | 1:7:A:LEU:HD23  | 20                  | 0.18     | 0.07                | 0.14       |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG11 | 20                  | 0.18     | 0.02                | 0.18       |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG12 | 20                  | 0.18     | 0.02                | 0.18       |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG13 | 20                  | 0.18     | 0.02                | 0.18       |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG21 | 20                  | 0.18     | 0.02                | 0.18       |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG22 | 20                  | 0.18     | 0.02                | 0.18       |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG23 | 20                  | 0.18     | 0.02                | 0.18       |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG11 | 20                  | 0.18     | 0.02                | 0.18       |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG12 | 20                  | 0.18     | 0.02                | 0.18       |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG13 | 20                  | 0.18     | 0.02                | 0.18       |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG21 | 20                  | 0.18     | 0.02                | 0.18       |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG22 | 20                  | 0.18     | 0.02                | 0.18       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG23 | 20                  | 0.18     | 0.02                | 0.18       |
| (1,1669) | 1:76:A:LEU:HD11 | 1:80:A:VAL:HB   | 20                  | 0.17     | 0.02                | 0.18       |
| (1,1669) | 1:76:A:LEU:HD12 | 1:80:A:VAL:HB   | 20                  | 0.17     | 0.02                | 0.18       |
| (1,1669) | 1:76:A:LEU:HD13 | 1:80:A:VAL:HB   | 20                  | 0.17     | 0.02                | 0.18       |
| (1,1669) | 1:76:A:LEU:HD21 | 1:80:A:VAL:HB   | 20                  | 0.17     | 0.02                | 0.18       |
| (1,1669) | 1:76:A:LEU:HD22 | 1:80:A:VAL:HB   | 20                  | 0.17     | 0.02                | 0.18       |
| (1,1669) | 1:76:A:LEU:HD23 | 1:80:A:VAL:HB   | 20                  | 0.17     | 0.02                | 0.18       |
| (1,1454) | 1:66:A:ILE:HA   | 1:67:A:PHE:H    | 20                  | 0.17     | 0.01                | 0.17       |
| (1,1168) | 1:52:A:HIS:HD2  | 1:52:A:HIS:HB2  | 20                  | 0.17     | 0.01                | 0.17       |
| (1,1168) | 1:52:A:HIS:HD2  | 1:52:A:HIS:HB3  | 20                  | 0.17     | 0.01                | 0.17       |
| (1,1762) | 1:82:A:TYR:HE1  | 1:82:A:TYR:H    | 20                  | 0.16     | 0.02                | 0.17       |
| (1,1762) | 1:82:A:TYR:HE2  | 1:82:A:TYR:H    | 20                  | 0.16     | 0.02                | 0.17       |
| (1,20)   | 1:2:A:ALA:HA    | 1:5:A:GLY:H     | 20                  | 0.16     | 0.02                | 0.16       |
| (1,339)  | 1:12:A:THR:HG21 | 1:46:A:PHE:HD1  | 20                  | 0.15     | 0.02                | 0.14       |
| (1,339)  | 1:12:A:THR:HG21 | 1:46:A:PHE:HD2  | 20                  | 0.15     | 0.02                | 0.14       |
| (1,339)  | 1:12:A:THR:HG22 | 1:46:A:PHE:HD1  | 20                  | 0.15     | 0.02                | 0.14       |
| (1,339)  | 1:12:A:THR:HG22 | 1:46:A:PHE:HD2  | 20                  | 0.15     | 0.02                | 0.14       |
| (1,339)  | 1:12:A:THR:HG23 | 1:46:A:PHE:HD1  | 20                  | 0.15     | 0.02                | 0.14       |
| (1,339)  | 1:12:A:THR:HG23 | 1:46:A:PHE:HD2  | 20                  | 0.15     | 0.02                | 0.14       |
| (1,1355) | 1:63:A:ILE:HB   | 1:63:A:ILE:H    | 20                  | 0.15     | 0.01                | 0.15       |
| (1,669)  | 1:27:A:CYS:HB2  | 1:30:A:ASP:H    | 20                  | 0.14     | 0.03                | 0.15       |
| (1,669)  | 1:27:A:CYS:HB3  | 1:30:A:ASP:H    | 20                  | 0.14     | 0.03                | 0.15       |
| (1,997)  | 1:45:A:TRP:HA   | 1:50:A:GLU:H    | 20                  | 0.14     | 0.02                | 0.15       |
| (1,1233) | 1:55:A:LEU:HG   | 1:63:A:ILE:HB   | 20                  | 0.14     | 0.02                | 0.15       |
| (1,1794) | 1:83:A:ARG:HG2  | 1:84:A:THR:H    | 20                  | 0.14     | 0.03                | 0.14       |
| (1,1794) | 1:83:A:ARG:HG3  | 1:84:A:THR:H    | 20                  | 0.14     | 0.03                | 0.14       |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG21 | 19                  | 0.2      | 0.04                | 0.19       |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG22 | 19                  | 0.2      | 0.04                | 0.19       |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG23 | 19                  | 0.2      | 0.04                | 0.19       |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG21 | 19                  | 0.2      | 0.04                | 0.19       |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG22 | 19                  | 0.2      | 0.04                | 0.19       |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG23 | 19                  | 0.2      | 0.04                | 0.19       |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG21 | 19                  | 0.2      | 0.04                | 0.19       |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG22 | 19                  | 0.2      | 0.04                | 0.19       |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG23 | 19                  | 0.2      | 0.04                | 0.19       |
| (1,1273) | 1:58:A:ASP:HA   | 1:59:A:ASN:HD21 | 19                  | 0.19     | 0.07                | 0.18       |
| (1,1273) | 1:58:A:ASP:HA   | 1:59:A:ASN:HD22 | 19                  | 0.19     | 0.07                | 0.18       |
| (1,1437) | 1:65:A:HIS:HA   | 1:68:A:GLU:H    | 19                  | 0.19     | 0.05                | 0.19       |
| (1,1428) | 1:65:A:HIS:HD2  | 1:66:A:ILE:HG12 | 19                  | 0.17     | 0.04                | 0.17       |
| (1,1428) | 1:65:A:HIS:HD2  | 1:66:A:ILE:HG13 | 19                  | 0.17     | 0.04                | 0.17       |
| (1,432)  | 1:16:A:THR:HG21 | 1:19:A:ASP:HB2  | 19                  | 0.16     | 0.03                | 0.15       |
| (1,432)  | 1:16:A:THR:HG21 | 1:19:A:ASP:HB3  | 19                  | 0.16     | 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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,432)  | 1:16:A:THR:HG22 | 1:19:A:ASP:HB2  | 19                  | 0.16     | 0.03                | 0.15       |
| (1,432)  | 1:16:A:THR:HG22 | 1:19:A:ASP:HB3  | 19                  | 0.16     | 0.03                | 0.15       |
| (1,432)  | 1:16:A:THR:HG23 | 1:19:A:ASP:HB2  | 19                  | 0.16     | 0.03                | 0.15       |
| (1,432)  | 1:16:A:THR:HG23 | 1:19:A:ASP:HB3  | 19                  | 0.16     | 0.03                | 0.15       |
| (1,425)  | 1:16:A:THR:HG21 | 1:18:A:GLU:H    | 19                  | 0.16     | 0.03                | 0.15       |
| (1,425)  | 1:16:A:THR:HG22 | 1:18:A:GLU:H    | 19                  | 0.16     | 0.03                | 0.15       |
| (1,425)  | 1:16:A:THR:HG23 | 1:18:A:GLU:H    | 19                  | 0.16     | 0.03                | 0.15       |
| (1,420)  | 1:16:A:THR:HG21 | 1:17:A:LEU:H    | 19                  | 0.15     | 0.03                | 0.14       |
| (1,420)  | 1:16:A:THR:HG22 | 1:17:A:LEU:H    | 19                  | 0.15     | 0.03                | 0.14       |
| (1,420)  | 1:16:A:THR:HG23 | 1:17:A:LEU:H    | 19                  | 0.15     | 0.03                | 0.14       |
| (1,127)  | 1:6:A:THR:HB    | 1:9:A:GLN:HG2   | 19                  | 0.14     | 0.02                | 0.14       |
| (1,127)  | 1:6:A:THR:HB    | 1:9:A:GLN:HG3   | 19                  | 0.14     | 0.02                | 0.14       |
| (1,772)  | 1:31:A:ILE:HG21 | 1:49:A:LEU:HA   | 18                  | 0.18     | 0.04                | 0.18       |
| (1,772)  | 1:31:A:ILE:HG22 | 1:49:A:LEU:HA   | 18                  | 0.18     | 0.04                | 0.18       |
| (1,772)  | 1:31:A:ILE:HG23 | 1:49:A:LEU:HA   | 18                  | 0.18     | 0.04                | 0.18       |
| (1,245)  | 1:9:A:GLN:HE21  | 1:12:A:THR:HG21 | 18                  | 0.16     | 0.02                | 0.16       |
| (1,245)  | 1:9:A:GLN:HE21  | 1:12:A:THR:HG22 | 18                  | 0.16     | 0.02                | 0.16       |
| (1,245)  | 1:9:A:GLN:HE21  | 1:12:A:THR:HG23 | 18                  | 0.16     | 0.02                | 0.16       |
| (1,245)  | 1:9:A:GLN:HE22  | 1:12:A:THR:HG21 | 18                  | 0.16     | 0.02                | 0.16       |
| (1,245)  | 1:9:A:GLN:HE22  | 1:12:A:THR:HG22 | 18                  | 0.16     | 0.02                | 0.16       |
| (1,245)  | 1:9:A:GLN:HE22  | 1:12:A:THR:HG23 | 18                  | 0.16     | 0.02                | 0.16       |
| (1,855)  | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD11 | 18                  | 0.15     | 0.04                | 0.15       |
| (1,855)  | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD12 | 18                  | 0.15     | 0.04                | 0.15       |
| (1,855)  | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD13 | 18                  | 0.15     | 0.04                | 0.15       |
| (1,855)  | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD11 | 18                  | 0.15     | 0.04                | 0.15       |
| (1,855)  | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD12 | 18                  | 0.15     | 0.04                | 0.15       |
| (1,855)  | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD13 | 18                  | 0.15     | 0.04                | 0.15       |
| (1,1888) | 1:89:A:ILE:HG21 | 1:89:A:ILE:H    | 18                  | 0.14     | 0.02                | 0.14       |
| (1,1888) | 1:89:A:ILE:HG22 | 1:89:A:ILE:H    | 18                  | 0.14     | 0.02                | 0.14       |
| (1,1888) | 1:89:A:ILE:HG23 | 1:89:A:ILE:H    | 18                  | 0.14     | 0.02                | 0.14       |
| (1,1255) | 1:57:A:LYS:HA   | 1:57:A:LYS:HG2  | 18                  | 0.14     | 0.02                | 0.14       |
| (1,1255) | 1:57:A:LYS:HA   | 1:57:A:LYS:HG3  | 18                  | 0.14     | 0.02                | 0.14       |
| (1,1439) | 1:65:A:HIS:HA   | 1:69:A:ILE:H    | 18                  | 0.14     | 0.02                | 0.13       |
| (1,124)  | 1:6:A:THR:HA    | 1:9:A:GLN:HG2   | 18                  | 0.13     | 0.02                | 0.14       |
| (1,124)  | 1:6:A:THR:HA    | 1:9:A:GLN:HG3   | 18                  | 0.13     | 0.02                | 0.14       |
| (1,555)  | 1:22:A:GLN:HA   | 1:23:A:LEU:H    | 18                  | 0.13     | 0.01                | 0.12       |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD2  | 17                  | 0.19     | 0.06                | 0.15       |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD3  | 17                  | 0.19     | 0.06                | 0.15       |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD2  | 17                  | 0.19     | 0.06                | 0.15       |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD3  | 17                  | 0.19     | 0.06                | 0.15       |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD2  | 17                  | 0.19     | 0.06                | 0.15       |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD3  | 17                  | 0.19     | 0.06                | 0.15       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1256) | 1:57:A:LYS:HA   | 1:57:A:LYS:HD2  | 17                  | 0.14     | 0.03                | 0.14       |
| (1,1256) | 1:57:A:LYS:HA   | 1:57:A:LYS:HD3  | 17                  | 0.14     | 0.03                | 0.14       |
| (1,1516) | 1:67:A:PHE:H    | 1:76:A:LEU:HG   | 17                  | 0.13     | 0.02                | 0.13       |
| (1,296)  | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD11 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD12 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD13 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD21 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD22 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD23 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD11 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD12 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD13 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD21 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD22 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD23 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD11 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD12 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD13 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD21 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD22 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD23 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD11 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD12 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD13 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD21 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD22 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD23 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD11 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD12 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD13 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD21 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD22 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD23 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD11 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD12 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD13 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD21 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD22 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,296)  | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD23 | 16                  | 0.18     | 0.04                | 0.18       |
| (1,1319) | 1:61:A:SER:HA   | 1:63:A:ILE:HG21 | 16                  | 0.14     | 0.03                | 0.14       |
| (1,1319) | 1:61:A:SER:HA   | 1:63:A:ILE:HG22 | 16                  | 0.14     | 0.03                | 0.14       |
| (1,1319) | 1:61:A:SER:HA   | 1:63:A:ILE:HG23 | 16                  | 0.14     | 0.03                | 0.14       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,285)  | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG21 | 16                  | 0.13     | 0.02                | 0.13       |
| (1,285)  | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG22 | 16                  | 0.13     | 0.02                | 0.13       |
| (1,285)  | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG23 | 16                  | 0.13     | 0.02                | 0.13       |
| (1,285)  | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG21 | 16                  | 0.13     | 0.02                | 0.13       |
| (1,285)  | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG22 | 16                  | 0.13     | 0.02                | 0.13       |
| (1,285)  | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG23 | 16                  | 0.13     | 0.02                | 0.13       |
| (1,724)  | 1:31:A:ILE:HD11 | 1:31:A:ILE:H    | 16                  | 0.13     | 0.01                | 0.13       |
| (1,724)  | 1:31:A:ILE:HD12 | 1:31:A:ILE:H    | 16                  | 0.13     | 0.01                | 0.13       |
| (1,724)  | 1:31:A:ILE:HD13 | 1:31:A:ILE:H    | 16                  | 0.13     | 0.01                | 0.13       |
| (1,926)  | 1:41:A:THR:HB   | 1:42:A:GLY:H    | 16                  | 0.13     | 0.02                | 0.12       |
| (1,1129) | 1:49:A:LEU:HG   | 1:62:A:TYR:HD1  | 15                  | 0.24     | 0.06                | 0.26       |
| (1,1129) | 1:49:A:LEU:HG   | 1:62:A:TYR:HD2  | 15                  | 0.24     | 0.06                | 0.26       |
| (1,743)  | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD2  | 15                  | 0.16     | 0.04                | 0.17       |
| (1,743)  | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD3  | 15                  | 0.16     | 0.04                | 0.17       |
| (1,743)  | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD2  | 15                  | 0.16     | 0.04                | 0.17       |
| (1,743)  | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD3  | 15                  | 0.16     | 0.04                | 0.17       |
| (1,743)  | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD2  | 15                  | 0.16     | 0.04                | 0.17       |
| (1,743)  | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD3  | 15                  | 0.16     | 0.04                | 0.17       |
| (1,982)  | 1:45:A:TRP:HE1  | 1:46:A:PHE:HA   | 15                  | 0.13     | 0.01                | 0.13       |
| (1,736)  | 1:31:A:ILE:HB   | 1:32:A:PRO:HA   | 15                  | 0.12     | 0.02                | 0.12       |
| (1,1292) | 1:60:A:LEU:HA   | 1:60:A:LEU:HD11 | 14                  | 0.13     | 0.02                | 0.12       |
| (1,1292) | 1:60:A:LEU:HA   | 1:60:A:LEU:HD12 | 14                  | 0.13     | 0.02                | 0.12       |
| (1,1292) | 1:60:A:LEU:HA   | 1:60:A:LEU:HD13 | 14                  | 0.13     | 0.02                | 0.12       |
| (1,1292) | 1:60:A:LEU:HA   | 1:60:A:LEU:HD21 | 14                  | 0.13     | 0.02                | 0.12       |
| (1,1292) | 1:60:A:LEU:HA   | 1:60:A:LEU:HD22 | 14                  | 0.13     | 0.02                | 0.12       |
| (1,1292) | 1:60:A:LEU:HA   | 1:60:A:LEU:HD23 | 14                  | 0.13     | 0.02                | 0.12       |
| (1,204)  | 1:8:A:LEU:HB2   | 1:46:A:PHE:HE1  | 14                  | 0.12     | 0.01                | 0.12       |
| (1,204)  | 1:8:A:LEU:HB2   | 1:46:A:PHE:HE2  | 14                  | 0.12     | 0.01                | 0.12       |
| (1,204)  | 1:8:A:LEU:HB3   | 1:46:A:PHE:HE1  | 14                  | 0.12     | 0.01                | 0.12       |
| (1,204)  | 1:8:A:LEU:HB3   | 1:46:A:PHE:HE2  | 14                  | 0.12     | 0.01                | 0.12       |
| (1,476)  | 1:19:A:ASP:H    | 1:20:A:LEU:H    | 14                  | 0.12     | 0.02                | 0.11       |
| (1,534)  | 1:20:A:LEU:HD11 | 1:67:A:PHE:HE1  | 13                  | 0.13     | 0.02                | 0.13       |
| (1,534)  | 1:20:A:LEU:HD11 | 1:67:A:PHE:HE2  | 13                  | 0.13     | 0.02                | 0.13       |
| (1,534)  | 1:20:A:LEU:HD12 | 1:67:A:PHE:HE1  | 13                  | 0.13     | 0.02                | 0.13       |
| (1,534)  | 1:20:A:LEU:HD12 | 1:67:A:PHE:HE2  | 13                  | 0.13     | 0.02                | 0.13       |
| (1,534)  | 1:20:A:LEU:HD13 | 1:67:A:PHE:HE1  | 13                  | 0.13     | 0.02                | 0.13       |
| (1,534)  | 1:20:A:LEU:HD13 | 1:67:A:PHE:HE2  | 13                  | 0.13     | 0.02                | 0.13       |
| (1,534)  | 1:20:A:LEU:HD21 | 1:67:A:PHE:HE1  | 13                  | 0.13     | 0.02                | 0.13       |
| (1,534)  | 1:20:A:LEU:HD21 | 1:67:A:PHE:HE2  | 13                  | 0.13     | 0.02                | 0.13       |
| (1,534)  | 1:20:A:LEU:HD22 | 1:67:A:PHE:HE1  | 13                  | 0.13     | 0.02                | 0.13       |
| (1,534)  | 1:20:A:LEU:HD22 | 1:67:A:PHE:HE2  | 13                  | 0.13     | 0.02                | 0.13       |
| (1,534)  | 1:20:A:LEU:HD23 | 1:67:A:PHE:HE1  | 13                  | 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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,534)  | 1:20:A:LEU:HD23 | 1:67:A:PHE:HE2  | 13                  | 0.13     | 0.02                | 0.13       |
| (1,1062) | 1:47:A:SER:HA   | 1:51:A:SER:H    | 13                  | 0.13     | 0.02                | 0.13       |
| (1,405)  | 1:15:A:ILE:HD11 | 1:43:A:SER:H    | 13                  | 0.13     | 0.02                | 0.13       |
| (1,405)  | 1:15:A:ILE:HD12 | 1:43:A:SER:H    | 13                  | 0.13     | 0.02                | 0.13       |
| (1,405)  | 1:15:A:ILE:HD13 | 1:43:A:SER:H    | 13                  | 0.13     | 0.02                | 0.13       |
| (1,1223) | 1:55:A:LEU:HG   | 1:56:A:ASP:HA   | 13                  | 0.13     | 0.02                | 0.12       |
| (1,761)  | 1:31:A:ILE:HD11 | 1:45:A:TRP:HD1  | 13                  | 0.12     | 0.01                | 0.11       |
| (1,761)  | 1:31:A:ILE:HD12 | 1:45:A:TRP:HD1  | 13                  | 0.12     | 0.01                | 0.11       |
| (1,761)  | 1:31:A:ILE:HD13 | 1:45:A:TRP:HD1  | 13                  | 0.12     | 0.01                | 0.11       |
| (1,846)  | 1:37:A:GLU:HA   | 1:38:A:GLU:H    | 12                  | 0.19     | 0.02                | 0.19       |
| (1,844)  | 1:37:A:GLU:H    | 1:38:A:GLU:H    | 12                  | 0.18     | 0.02                | 0.18       |
| (1,1207) | 1:54:A:LYS:HG2  | 1:62:A:TYR:HE1  | 12                  | 0.13     | 0.03                | 0.13       |
| (1,1207) | 1:54:A:LYS:HG2  | 1:62:A:TYR:HE2  | 12                  | 0.13     | 0.03                | 0.13       |
| (1,1207) | 1:54:A:LYS:HG3  | 1:62:A:TYR:HE1  | 12                  | 0.13     | 0.03                | 0.13       |
| (1,1207) | 1:54:A:LYS:HG3  | 1:62:A:TYR:HE2  | 12                  | 0.13     | 0.03                | 0.13       |
| (1,604)  | 1:23:A:LEU:HG   | 1:66:A:ILE:HG21 | 12                  | 0.13     | 0.01                | 0.13       |
| (1,604)  | 1:23:A:LEU:HG   | 1:66:A:ILE:HG22 | 12                  | 0.13     | 0.01                | 0.13       |
| (1,604)  | 1:23:A:LEU:HG   | 1:66:A:ILE:HG23 | 12                  | 0.13     | 0.01                | 0.13       |
| (1,1777) | 1:82:A:TYR:HD1  | 1:85:A:ARG:HG2  | 10                  | 0.15     | 0.03                | 0.15       |
| (1,1777) | 1:82:A:TYR:HD1  | 1:85:A:ARG:HG3  | 10                  | 0.15     | 0.03                | 0.15       |
| (1,1777) | 1:82:A:TYR:HD2  | 1:85:A:ARG:HG2  | 10                  | 0.15     | 0.03                | 0.15       |
| (1,1777) | 1:82:A:TYR:HD2  | 1:85:A:ARG:HG3  | 10                  | 0.15     | 0.03                | 0.15       |
| (1,1267) | 1:57:A:LYS:HD2  | 1:59:A:ASN:H    | 10                  | 0.14     | 0.02                | 0.14       |
| (1,1267) | 1:57:A:LYS:HD3  | 1:59:A:ASN:H    | 10                  | 0.14     | 0.02                | 0.14       |
| (1,1349) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HD11 | 10                  | 0.14     | 0.02                | 0.14       |
| (1,1349) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HD12 | 10                  | 0.14     | 0.02                | 0.14       |
| (1,1349) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HD13 | 10                  | 0.14     | 0.02                | 0.14       |
| (1,1349) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HD11 | 10                  | 0.14     | 0.02                | 0.14       |
| (1,1349) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HD12 | 10                  | 0.14     | 0.02                | 0.14       |
| (1,1349) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HD13 | 10                  | 0.14     | 0.02                | 0.14       |
| (1,1609) | 1:73:A:PRO:HA   | 1:73:A:PRO:HG2  | 10                  | 0.14     | 0.01                | 0.13       |
| (1,1609) | 1:73:A:PRO:HA   | 1:73:A:PRO:HG3  | 10                  | 0.14     | 0.01                | 0.13       |
| (1,512)  | 1:20:A:LEU:HB2  | 1:24:A:LYS:HG2  | 9                   | 0.2      | 0.03                | 0.21       |
| (1,512)  | 1:20:A:LEU:HB2  | 1:24:A:LYS:HG3  | 9                   | 0.2      | 0.03                | 0.21       |
| (1,512)  | 1:20:A:LEU:HB3  | 1:24:A:LYS:HG2  | 9                   | 0.2      | 0.03                | 0.21       |
| (1,512)  | 1:20:A:LEU:HB3  | 1:24:A:LYS:HG3  | 9                   | 0.2      | 0.03                | 0.21       |
| (1,93)   | 1:4:A:TYR:HA    | 1:82:A:TYR:HE1  | 9                   | 0.15     | 0.04                | 0.15       |
| (1,93)   | 1:4:A:TYR:HA    | 1:82:A:TYR:HE2  | 9                   | 0.15     | 0.04                | 0.15       |
| (1,1228) | 1:55:A:LEU:HG   | 1:59:A:ASN:HD21 | 9                   | 0.14     | 0.03                | 0.12       |
| (1,1228) | 1:55:A:LEU:HG   | 1:59:A:ASN:HD22 | 9                   | 0.14     | 0.03                | 0.12       |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD11 | 9                   | 0.12     | 0.01                | 0.13       |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD12 | 9                   | 0.12     | 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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD13 | 9                   | 0.12     | 0.01                | 0.13       |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD21 | 9                   | 0.12     | 0.01                | 0.13       |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD22 | 9                   | 0.12     | 0.01                | 0.13       |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD23 | 9                   | 0.12     | 0.01                | 0.13       |
| (1,1576) | 1:71:A:ARG:HA   | 1:71:A:ARG:HG2  | 9                   | 0.12     | 0.01                | 0.12       |
| (1,1576) | 1:71:A:ARG:HA   | 1:71:A:ARG:HG3  | 9                   | 0.12     | 0.01                | 0.12       |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG11 | 9                   | 0.11     | 0.01                | 0.12       |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG12 | 9                   | 0.11     | 0.01                | 0.12       |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG13 | 9                   | 0.11     | 0.01                | 0.12       |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG21 | 9                   | 0.11     | 0.01                | 0.12       |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG22 | 9                   | 0.11     | 0.01                | 0.12       |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG23 | 9                   | 0.11     | 0.01                | 0.12       |
| (1,138)  | 1:7:A:LEU:HA    | 1:7:A:LEU:HG    | 8                   | 0.32     | 0.01                | 0.32       |
| (1,1340) | 1:62:A:TYR:HD1  | 1:63:A:ILE:H    | 8                   | 0.25     | 0.02                | 0.25       |
| (1,1340) | 1:62:A:TYR:HD2  | 1:63:A:ILE:H    | 8                   | 0.25     | 0.02                | 0.25       |
| (1,627)  | 1:24:A:LYS:HG2  | 1:45:A:TRP:HD1  | 8                   | 0.18     | 0.04                | 0.17       |
| (1,627)  | 1:24:A:LYS:HG3  | 1:45:A:TRP:HD1  | 8                   | 0.18     | 0.04                | 0.17       |
| (1,1194) | 1:54:A:LYS:HD2  | 1:54:A:LYS:H    | 8                   | 0.17     | 0.06                | 0.17       |
| (1,1194) | 1:54:A:LYS:HD3  | 1:54:A:LYS:H    | 8                   | 0.17     | 0.06                | 0.17       |
| (1,566)  | 1:22:A:GLN:HG2  | 1:25:A:SER:HB2  | 8                   | 0.16     | 0.04                | 0.17       |
| (1,566)  | 1:22:A:GLN:HG2  | 1:25:A:SER:HB3  | 8                   | 0.16     | 0.04                | 0.17       |
| (1,566)  | 1:22:A:GLN:HG3  | 1:25:A:SER:HB2  | 8                   | 0.16     | 0.04                | 0.17       |
| (1,566)  | 1:22:A:GLN:HG3  | 1:25:A:SER:HB3  | 8                   | 0.16     | 0.04                | 0.17       |
| (1,6)    | 1:1:A:MET:HA    | 1:3:A:GLU:H     | 8                   | 0.15     | 0.03                | 0.14       |
| (1,147)  | 1:7:A:LEU:HG    | 1:8:A:LEU:HD11  | 8                   | 0.14     | 0.01                | 0.14       |
| (1,147)  | 1:7:A:LEU:HG    | 1:8:A:LEU:HD12  | 8                   | 0.14     | 0.01                | 0.14       |
| (1,147)  | 1:7:A:LEU:HG    | 1:8:A:LEU:HD13  | 8                   | 0.14     | 0.01                | 0.14       |
| (1,147)  | 1:7:A:LEU:HG    | 1:8:A:LEU:HD21  | 8                   | 0.14     | 0.01                | 0.14       |
| (1,147)  | 1:7:A:LEU:HG    | 1:8:A:LEU:HD22  | 8                   | 0.14     | 0.01                | 0.14       |
| (1,147)  | 1:7:A:LEU:HG    | 1:8:A:LEU:HD23  | 8                   | 0.14     | 0.01                | 0.14       |
| (1,1018) | 1:46:A:PHE:HD1  | 1:46:A:PHE:H    | 8                   | 0.13     | 0.02                | 0.12       |
| (1,1018) | 1:46:A:PHE:HD2  | 1:46:A:PHE:H    | 8                   | 0.13     | 0.02                | 0.12       |
| (1,783)  | 1:32:A:PRO:HD2  | 1:35:A:LYS:HG2  | 8                   | 0.12     | 0.02                | 0.12       |
| (1,783)  | 1:32:A:PRO:HD2  | 1:35:A:LYS:HG3  | 8                   | 0.12     | 0.02                | 0.12       |
| (1,783)  | 1:32:A:PRO:HD3  | 1:35:A:LYS:HG2  | 8                   | 0.12     | 0.02                | 0.12       |
| (1,783)  | 1:32:A:PRO:HD3  | 1:35:A:LYS:HG3  | 8                   | 0.12     | 0.02                | 0.12       |
| (1,1900) | 1:89:A:ILE:HG21 | 1:90:A:SER:HB2  | 8                   | 0.12     | 0.02                | 0.12       |
| (1,1900) | 1:89:A:ILE:HG21 | 1:90:A:SER:HB3  | 8                   | 0.12     | 0.02                | 0.12       |
| (1,1900) | 1:89:A:ILE:HG22 | 1:90:A:SER:HB2  | 8                   | 0.12     | 0.02                | 0.12       |
| (1,1900) | 1:89:A:ILE:HG22 | 1:90:A:SER:HB3  | 8                   | 0.12     | 0.02                | 0.12       |
| (1,1900) | 1:89:A:ILE:HG23 | 1:90:A:SER:HB2  | 8                   | 0.12     | 0.02                | 0.12       |
| (1,1900) | 1:89:A:ILE:HG23 | 1:90:A:SER:HB3  | 8                   | 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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1680) | 1:77:A:THR:HG21 | 1:78:A:MET:HG2  | 8                   | 0.12     | 0.02                | 0.11       |
| (1,1680) | 1:77:A:THR:HG21 | 1:78:A:MET:HG3  | 8                   | 0.12     | 0.02                | 0.11       |
| (1,1680) | 1:77:A:THR:HG22 | 1:78:A:MET:HG2  | 8                   | 0.12     | 0.02                | 0.11       |
| (1,1680) | 1:77:A:THR:HG22 | 1:78:A:MET:HG3  | 8                   | 0.12     | 0.02                | 0.11       |
| (1,1680) | 1:77:A:THR:HG23 | 1:78:A:MET:HG2  | 8                   | 0.12     | 0.02                | 0.11       |
| (1,1680) | 1:77:A:THR:HG23 | 1:78:A:MET:HG3  | 8                   | 0.12     | 0.02                | 0.11       |
| (1,438)  | 1:17:A:LEU:HA   | 1:17:A:LEU:HG   | 7                   | 0.28     | 0.03                | 0.27       |
| (1,1825) | 1:84:A:THR:HB   | 1:87:A:LEU:HG   | 7                   | 0.19     | 0.04                | 0.21       |
| (1,483)  | 1:19:A:ASP:HA   | 1:22:A:GLN:HE21 | 7                   | 0.18     | 0.04                | 0.19       |
| (1,483)  | 1:19:A:ASP:HA   | 1:22:A:GLN:HE22 | 7                   | 0.18     | 0.04                | 0.19       |
| (1,1211) | 1:54:A:LYS:HB2  | 1:62:A:TYR:H    | 7                   | 0.17     | 0.02                | 0.16       |
| (1,1211) | 1:54:A:LYS:HB3  | 1:62:A:TYR:H    | 7                   | 0.17     | 0.02                | 0.16       |
| (1,10)   | 1:1:A:MET:HA    | 1:57:A:LYS:HD2  | 7                   | 0.15     | 0.04                | 0.15       |
| (1,10)   | 1:1:A:MET:HA    | 1:57:A:LYS:HD3  | 7                   | 0.15     | 0.04                | 0.15       |
| (1,418)  | 1:16:A:THR:HB   | 1:16:A:THR:H    | 7                   | 0.12     | 0.01                | 0.12       |
| (1,373)  | 1:14:A:ASN:HB2  | 1:75:A:LEU:HG   | 7                   | 0.12     | 0.02                | 0.12       |
| (1,373)  | 1:14:A:ASN:HB3  | 1:75:A:LEU:HG   | 7                   | 0.12     | 0.02                | 0.12       |
| (1,1834) | 1:85:A:ARG:HD2  | 1:86:A:VAL:HA   | 7                   | 0.12     | 0.01                | 0.12       |
| (1,1834) | 1:85:A:ARG:HD3  | 1:86:A:VAL:HA   | 7                   | 0.12     | 0.01                | 0.12       |
| (1,1538) | 1:68:A:GLU:HA   | 1:71:A:ARG:HD2  | 7                   | 0.11     | 0.01                | 0.11       |
| (1,1538) | 1:68:A:GLU:HA   | 1:71:A:ARG:HD3  | 7                   | 0.11     | 0.01                | 0.11       |
| (1,923)  | 1:41:A:THR:HB   | 1:41:A:THR:H    | 7                   | 0.11     | 0.01                | 0.11       |
| (1,1193) | 1:53:A:ASN:H    | 1:55:A:LEU:H    | 7                   | 0.11     | 0.01                | 0.1        |
| (1,918)  | 1:40:A:THR:HA   | 1:41:A:THR:H    | 6                   | 0.18     | 0.07                | 0.15       |
| (1,1541) | 1:68:A:GLU:HG2  | 1:76:A:LEU:HD11 | 6                   | 0.16     | 0.03                | 0.17       |
| (1,1541) | 1:68:A:GLU:HG2  | 1:76:A:LEU:HD12 | 6                   | 0.16     | 0.03                | 0.17       |
| (1,1541) | 1:68:A:GLU:HG2  | 1:76:A:LEU:HD13 | 6                   | 0.16     | 0.03                | 0.17       |
| (1,1541) | 1:68:A:GLU:HG2  | 1:76:A:LEU:HD21 | 6                   | 0.16     | 0.03                | 0.17       |
| (1,1541) | 1:68:A:GLU:HG2  | 1:76:A:LEU:HD22 | 6                   | 0.16     | 0.03                | 0.17       |
| (1,1541) | 1:68:A:GLU:HG2  | 1:76:A:LEU:HD23 | 6                   | 0.16     | 0.03                | 0.17       |
| (1,1541) | 1:68:A:GLU:HG3  | 1:76:A:LEU:HD11 | 6                   | 0.16     | 0.03                | 0.17       |
| (1,1541) | 1:68:A:GLU:HG3  | 1:76:A:LEU:HD12 | 6                   | 0.16     | 0.03                | 0.17       |
| (1,1541) | 1:68:A:GLU:HG3  | 1:76:A:LEU:HD13 | 6                   | 0.16     | 0.03                | 0.17       |
| (1,1541) | 1:68:A:GLU:HG3  | 1:76:A:LEU:HD21 | 6                   | 0.16     | 0.03                | 0.17       |
| (1,1541) | 1:68:A:GLU:HG3  | 1:76:A:LEU:HD22 | 6                   | 0.16     | 0.03                | 0.17       |
| (1,1541) | 1:68:A:GLU:HG3  | 1:76:A:LEU:HD23 | 6                   | 0.16     | 0.03                | 0.17       |
| (1,1597) | 1:72:A:ARG:HG2  | 1:74:A:ASP:H    | 6                   | 0.14     | 0.02                | 0.14       |
| (1,1597) | 1:72:A:ARG:HG3  | 1:74:A:ASP:H    | 6                   | 0.14     | 0.02                | 0.14       |
| (1,1277) | 1:58:A:ASP:H    | 1:60:A:LEU:H    | 6                   | 0.13     | 0.02                | 0.12       |
| (1,1206) | 1:54:A:LYS:HB2  | 1:62:A:TYR:HE1  | 6                   | 0.12     | 0.02                | 0.12       |
| (1,1206) | 1:54:A:LYS:HB2  | 1:62:A:TYR:HE2  | 6                   | 0.12     | 0.02                | 0.12       |
| (1,1206) | 1:54:A:LYS:HB3  | 1:62:A:TYR:HE1  | 6                   | 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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1206) | 1:54:A:LYS:HB3  | 1:62:A:TYR:HE2  | 6                   | 0.12     | 0.02                | 0.12       |
| (1,263)  | 1:10:A:ASP:H    | 1:14:A:ASN:H    | 6                   | 0.12     | 0.01                | 0.12       |
| (1,1445) | 1:66:A:ILE:HG12 | 1:66:A:ILE:H    | 6                   | 0.11     | 0.0                 | 0.11       |
| (1,1445) | 1:66:A:ILE:HG13 | 1:66:A:ILE:H    | 6                   | 0.11     | 0.0                 | 0.11       |
| (1,1525) | 1:68:A:GLU:HA   | 1:68:A:GLU:HG2  | 5                   | 0.15     | 0.01                | 0.15       |
| (1,1525) | 1:68:A:GLU:HA   | 1:68:A:GLU:HG3  | 5                   | 0.15     | 0.01                | 0.15       |
| (1,1796) | 1:83:A:ARG:HD2  | 1:84:A:THR:HG21 | 5                   | 0.14     | 0.04                | 0.12       |
| (1,1796) | 1:83:A:ARG:HD2  | 1:84:A:THR:HG22 | 5                   | 0.14     | 0.04                | 0.12       |
| (1,1796) | 1:83:A:ARG:HD2  | 1:84:A:THR:HG23 | 5                   | 0.14     | 0.04                | 0.12       |
| (1,1796) | 1:83:A:ARG:HD3  | 1:84:A:THR:HG21 | 5                   | 0.14     | 0.04                | 0.12       |
| (1,1796) | 1:83:A:ARG:HD3  | 1:84:A:THR:HG22 | 5                   | 0.14     | 0.04                | 0.12       |
| (1,1796) | 1:83:A:ARG:HD3  | 1:84:A:THR:HG23 | 5                   | 0.14     | 0.04                | 0.12       |
| (1,1745) | 1:80:A:VAL:HA   | 1:83:A:ARG:HD2  | 5                   | 0.13     | 0.02                | 0.13       |
| (1,1745) | 1:80:A:VAL:HA   | 1:83:A:ARG:HD3  | 5                   | 0.13     | 0.02                | 0.13       |
| (1,1010) | 1:45:A:TRP:HE1  | 1:66:A:ILE:HG12 | 5                   | 0.13     | 0.02                | 0.12       |
| (1,1010) | 1:45:A:TRP:HE1  | 1:66:A:ILE:HG13 | 5                   | 0.13     | 0.02                | 0.12       |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD11 | 5                   | 0.13     | 0.01                | 0.13       |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD12 | 5                   | 0.13     | 0.01                | 0.13       |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD13 | 5                   | 0.13     | 0.01                | 0.13       |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD21 | 5                   | 0.13     | 0.01                | 0.13       |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD22 | 5                   | 0.13     | 0.01                | 0.13       |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD23 | 5                   | 0.13     | 0.01                | 0.13       |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD11 | 5                   | 0.13     | 0.01                | 0.13       |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD12 | 5                   | 0.13     | 0.01                | 0.13       |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD13 | 5                   | 0.13     | 0.01                | 0.13       |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD21 | 5                   | 0.13     | 0.01                | 0.13       |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD22 | 5                   | 0.13     | 0.01                | 0.13       |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD23 | 5                   | 0.13     | 0.01                | 0.13       |
| (1,387)  | 1:15:A:ILE:HD11 | 1:19:A:ASP:H    | 5                   | 0.12     | 0.02                | 0.12       |
| (1,387)  | 1:15:A:ILE:HD12 | 1:19:A:ASP:H    | 5                   | 0.12     | 0.02                | 0.12       |
| (1,387)  | 1:15:A:ILE:HD13 | 1:19:A:ASP:H    | 5                   | 0.12     | 0.02                | 0.12       |
| (1,76)   | 1:4:A:TYR:HD1   | 1:56:A:ASP:HA   | 5                   | 0.12     | 0.02                | 0.11       |
| (1,76)   | 1:4:A:TYR:HD2   | 1:56:A:ASP:HA   | 5                   | 0.12     | 0.02                | 0.11       |
| (1,1838) | 1:85:A:ARG:H    | 1:86:A:VAL:HB   | 5                   | 0.11     | 0.01                | 0.11       |
| (1,1199) | 1:54:A:LYS:HA   | 1:54:A:LYS:HD2  | 4                   | 0.31     | 0.04                | 0.31       |
| (1,1199) | 1:54:A:LYS:HA   | 1:54:A:LYS:HD3  | 4                   | 0.31     | 0.04                | 0.31       |
| (1,1198) | 1:54:A:LYS:HA   | 1:54:A:LYS:HE2  | 4                   | 0.22     | 0.02                | 0.22       |
| (1,1198) | 1:54:A:LYS:HA   | 1:54:A:LYS:HE3  | 4                   | 0.22     | 0.02                | 0.22       |
| (1,1200) | 1:54:A:LYS:HA   | 1:54:A:LYS:HE2  | 4                   | 0.22     | 0.02                | 0.22       |
| (1,1200) | 1:54:A:LYS:HA   | 1:54:A:LYS:HE3  | 4                   | 0.22     | 0.02                | 0.22       |
| (1,80)   | 1:4:A:TYR:HD1   | 1:57:A:LYS:HB2  | 4                   | 0.14     | 0.02                | 0.14       |
| (1,80)   | 1:4:A:TYR:HD1   | 1:57:A:LYS:HB3  | 4                   | 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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,80)   | 1:4:A:TYR:HD2   | 1:57:A:LYS:HB2  | 4                   | 0.14     | 0.02                | 0.14       |
| (1,80)   | 1:4:A:TYR:HD2   | 1:57:A:LYS:HB3  | 4                   | 0.14     | 0.02                | 0.14       |
| (1,705)  | 1:29:A:GLU:HA   | 1:29:A:GLU:HG2  | 4                   | 0.13     | 0.03                | 0.12       |
| (1,705)  | 1:29:A:GLU:HA   | 1:29:A:GLU:HG3  | 4                   | 0.13     | 0.03                | 0.12       |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG11 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG12 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG13 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG21 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG22 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG23 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG11 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG12 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG13 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG21 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG22 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG23 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG11 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG12 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG13 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG21 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG22 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG23 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1324) | 1:61:A:SER:H    | 1:65:A:HIS:H    | 4                   | 0.12     | 0.02                | 0.12       |
| (1,1465) | 1:66:A:ILE:HD11 | 1:69:A:ILE:HA   | 4                   | 0.12     | 0.01                | 0.12       |
| (1,1465) | 1:66:A:ILE:HD12 | 1:69:A:ILE:HA   | 4                   | 0.12     | 0.01                | 0.12       |
| (1,1465) | 1:66:A:ILE:HD13 | 1:69:A:ILE:HA   | 4                   | 0.12     | 0.01                | 0.12       |
| (1,802)  | 1:35:A:LYS:HA   | 1:35:A:LYS:HD2  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,802)  | 1:35:A:LYS:HA   | 1:35:A:LYS:HD3  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,775)  | 1:32:A:PRO:HA   | 1:32:A:PRO:HG2  | 4                   | 0.12     | 0.0                 | 0.12       |
| (1,775)  | 1:32:A:PRO:HA   | 1:32:A:PRO:HG3  | 4                   | 0.12     | 0.0                 | 0.12       |
| (1,398)  | 1:15:A:ILE:HD11 | 1:23:A:LEU:HB2  | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,398)  | 1:15:A:ILE:HD11 | 1:23:A:LEU:HB3  | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,398)  | 1:15:A:ILE:HD12 | 1:23:A:LEU:HB2  | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,398)  | 1:15:A:ILE:HD12 | 1:23:A:LEU:HB3  | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,398)  | 1:15:A:ILE:HD13 | 1:23:A:LEU:HB2  | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,398)  | 1:15:A:ILE:HD13 | 1:23:A:LEU:HB3  | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,643)  | 1:26:A:ALA:HA   | 1:28:A:LYS:HB2  | 4                   | 0.1      | 0.0                 | 0.11       |
| (1,643)  | 1:26:A:ALA:HA   | 1:28:A:LYS:HB3  | 4                   | 0.1      | 0.0                 | 0.11       |
| (1,1879) | 1:88:A:LYS:HD2  | 1:88:A:LYS:HA   | 3                   | 0.26     | 0.04                | 0.28       |
| (1,1879) | 1:88:A:LYS:HD3  | 1:88:A:LYS:HA   | 3                   | 0.26     | 0.04                | 0.28       |
| (1,232)  | 1:9:A:GLN:HA    | 1:9:A:GLN:HG2   | 3                   | 0.16     | 0.03                | 0.15       |
| (1,232)  | 1:9:A:GLN:HA    | 1:9:A:GLN:HG3   | 3                   | 0.16     | 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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,843)  | 1:37:A:GLU:HA   | 1:37:A:GLU:HG2  | 3                   | 0.15     | 0.02                | 0.14       |
| (1,843)  | 1:37:A:GLU:HA   | 1:37:A:GLU:HG3  | 3                   | 0.15     | 0.02                | 0.14       |
| (1,792)  | 1:34:A:GLU:HA   | 1:34:A:GLU:HG2  | 3                   | 0.14     | 0.02                | 0.13       |
| (1,792)  | 1:34:A:GLU:HA   | 1:34:A:GLU:HG3  | 3                   | 0.14     | 0.02                | 0.13       |
| (1,25)   | 1:3:A:GLU:HG2   | 1:3:A:GLU:HA    | 3                   | 0.13     | 0.01                | 0.14       |
| (1,25)   | 1:3:A:GLU:HG3   | 1:3:A:GLU:HA    | 3                   | 0.13     | 0.01                | 0.14       |
| (1,335)  | 1:12:A:THR:HB   | 1:42:A:GLY:H    | 3                   | 0.13     | 0.02                | 0.13       |
| (1,901)  | 1:39:A:ILE:HG12 | 1:45:A:TRP:HD1  | 3                   | 0.13     | 0.02                | 0.13       |
| (1,901)  | 1:39:A:ILE:HG13 | 1:45:A:TRP:HD1  | 3                   | 0.13     | 0.02                | 0.13       |
| (1,557)  | 1:22:A:GLN:HE21 | 1:23:A:LEU:HA   | 3                   | 0.13     | 0.02                | 0.13       |
| (1,557)  | 1:22:A:GLN:HE22 | 1:23:A:LEU:HA   | 3                   | 0.13     | 0.02                | 0.13       |
| (1,1274) | 1:58:A:ASP:H    | 1:59:A:ASN:HD21 | 3                   | 0.13     | 0.04                | 0.11       |
| (1,1274) | 1:58:A:ASP:H    | 1:59:A:ASN:HD22 | 3                   | 0.13     | 0.04                | 0.11       |
| (1,1735) | 1:80:A:VAL:HG11 | 1:81:A:ASP:HA   | 3                   | 0.12     | 0.01                | 0.12       |
| (1,1735) | 1:80:A:VAL:HG12 | 1:81:A:ASP:HA   | 3                   | 0.12     | 0.01                | 0.12       |
| (1,1735) | 1:80:A:VAL:HG13 | 1:81:A:ASP:HA   | 3                   | 0.12     | 0.01                | 0.12       |
| (1,1735) | 1:80:A:VAL:HG21 | 1:81:A:ASP:HA   | 3                   | 0.12     | 0.01                | 0.12       |
| (1,1735) | 1:80:A:VAL:HG22 | 1:81:A:ASP:HA   | 3                   | 0.12     | 0.01                | 0.12       |
| (1,1735) | 1:80:A:VAL:HG23 | 1:81:A:ASP:HA   | 3                   | 0.12     | 0.01                | 0.12       |
| (1,487)  | 1:20:A:LEU:HG   | 1:20:A:LEU:H    | 3                   | 0.12     | 0.01                | 0.12       |
| (1,1874) | 1:87:A:LEU:HB2  | 1:89:A:ILE:HG21 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,1874) | 1:87:A:LEU:HB2  | 1:89:A:ILE:HG22 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,1874) | 1:87:A:LEU:HB2  | 1:89:A:ILE:HG23 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,1874) | 1:87:A:LEU:HB3  | 1:89:A:ILE:HG21 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,1874) | 1:87:A:LEU:HB3  | 1:89:A:ILE:HG22 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,1874) | 1:87:A:LEU:HB3  | 1:89:A:ILE:HG23 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,304)  | 1:11:A:LEU:HD11 | 1:75:A:LEU:HG   | 3                   | 0.12     | 0.01                | 0.12       |
| (1,304)  | 1:11:A:LEU:HD12 | 1:75:A:LEU:HG   | 3                   | 0.12     | 0.01                | 0.12       |
| (1,304)  | 1:11:A:LEU:HD13 | 1:75:A:LEU:HG   | 3                   | 0.12     | 0.01                | 0.12       |
| (1,304)  | 1:11:A:LEU:HD21 | 1:75:A:LEU:HG   | 3                   | 0.12     | 0.01                | 0.12       |
| (1,304)  | 1:11:A:LEU:HD22 | 1:75:A:LEU:HG   | 3                   | 0.12     | 0.01                | 0.12       |
| (1,304)  | 1:11:A:LEU:HD23 | 1:75:A:LEU:HG   | 3                   | 0.12     | 0.01                | 0.12       |
| (1,909)  | 1:39:A:ILE:HG12 | 1:48:A:PHE:H    | 3                   | 0.12     | 0.01                | 0.11       |
| (1,909)  | 1:39:A:ILE:HG13 | 1:48:A:PHE:H    | 3                   | 0.12     | 0.01                | 0.11       |
| (1,1399) | 1:64:A:GLU:HA   | 1:67:A:PHE:H    | 3                   | 0.12     | 0.01                | 0.11       |
| (1,1379) | 1:63:A:ILE:HD11 | 1:67:A:PHE:H    | 3                   | 0.11     | 0.01                | 0.11       |
| (1,1379) | 1:63:A:ILE:HD12 | 1:67:A:PHE:H    | 3                   | 0.11     | 0.01                | 0.11       |
| (1,1379) | 1:63:A:ILE:HD13 | 1:67:A:PHE:H    | 3                   | 0.11     | 0.01                | 0.11       |
| (1,459)  | 1:17:A:LEU:HG   | 1:40:A:THR:HB   | 3                   | 0.11     | 0.01                | 0.11       |
| (1,490)  | 1:20:A:LEU:HA   | 1:20:A:LEU:HG   | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1781) | 1:82:A:TYR:HB2  | 1:86:A:VAL:HG11 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1781) | 1:82:A:TYR:HB2  | 1:86:A:VAL:HG12 | 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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1781) | 1:82:A:TYR:HB2  | 1:86:A:VAL:HG13 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1781) | 1:82:A:TYR:HB2  | 1:86:A:VAL:HG21 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1781) | 1:82:A:TYR:HB2  | 1:86:A:VAL:HG22 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1781) | 1:82:A:TYR:HB2  | 1:86:A:VAL:HG23 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1781) | 1:82:A:TYR:HB3  | 1:86:A:VAL:HG11 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1781) | 1:82:A:TYR:HB3  | 1:86:A:VAL:HG12 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1781) | 1:82:A:TYR:HB3  | 1:86:A:VAL:HG13 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1781) | 1:82:A:TYR:HB3  | 1:86:A:VAL:HG21 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1781) | 1:82:A:TYR:HB3  | 1:86:A:VAL:HG22 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1781) | 1:82:A:TYR:HB3  | 1:86:A:VAL:HG23 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,675)  | 1:27:A:CYS:H    | 1:31:A:ILE:HB   | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,713)  | 1:29:A:GLU:HB2  | 1:31:A:ILE:H    | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,713)  | 1:29:A:GLU:HB3  | 1:31:A:ILE:H    | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,1250) | 1:56:A:ASP:H    | 1:59:A:ASN:HB2  | 2                   | 0.24     | 0.01                | 0.24       |
| (1,1250) | 1:56:A:ASP:H    | 1:59:A:ASN:HB3  | 2                   | 0.24     | 0.01                | 0.24       |
| (1,1251) | 1:56:A:ASP:H    | 1:59:A:ASN:HD21 | 2                   | 0.18     | 0.04                | 0.18       |
| (1,1251) | 1:56:A:ASP:H    | 1:59:A:ASN:HD22 | 2                   | 0.18     | 0.04                | 0.18       |
| (1,1259) | 1:57:A:LYS:HE2  | 1:58:A:ASP:H    | 2                   | 0.16     | 0.05                | 0.16       |
| (1,1259) | 1:57:A:LYS:HE3  | 1:58:A:ASP:H    | 2                   | 0.16     | 0.05                | 0.16       |
| (1,1264) | 1:57:A:LYS:HG2  | 1:58:A:ASP:HA   | 2                   | 0.15     | 0.02                | 0.15       |
| (1,1264) | 1:57:A:LYS:HG3  | 1:58:A:ASP:HA   | 2                   | 0.15     | 0.02                | 0.15       |
| (1,1246) | 1:56:A:ASP:H    | 1:59:A:ASN:H    | 2                   | 0.15     | 0.02                | 0.15       |
| (1,516)  | 1:20:A:LEU:HD11 | 1:39:A:ILE:HD11 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,516)  | 1:20:A:LEU:HD11 | 1:39:A:ILE:HD12 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,516)  | 1:20:A:LEU:HD11 | 1:39:A:ILE:HD13 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,516)  | 1:20:A:LEU:HD12 | 1:39:A:ILE:HD11 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,516)  | 1:20:A:LEU:HD12 | 1:39:A:ILE:HD12 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,516)  | 1:20:A:LEU:HD12 | 1:39:A:ILE:HD13 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,516)  | 1:20:A:LEU:HD13 | 1:39:A:ILE:HD11 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,516)  | 1:20:A:LEU:HD13 | 1:39:A:ILE:HD12 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,516)  | 1:20:A:LEU:HD13 | 1:39:A:ILE:HD13 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,516)  | 1:20:A:LEU:HD21 | 1:39:A:ILE:HD11 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,516)  | 1:20:A:LEU:HD21 | 1:39:A:ILE:HD12 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,516)  | 1:20:A:LEU:HD21 | 1:39:A:ILE:HD13 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,516)  | 1:20:A:LEU:HD22 | 1:39:A:ILE:HD11 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,516)  | 1:20:A:LEU:HD22 | 1:39:A:ILE:HD12 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,516)  | 1:20:A:LEU:HD22 | 1:39:A:ILE:HD13 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,516)  | 1:20:A:LEU:HD23 | 1:39:A:ILE:HD11 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,516)  | 1:20:A:LEU:HD23 | 1:39:A:ILE:HD12 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,516)  | 1:20:A:LEU:HD23 | 1:39:A:ILE:HD13 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,1823) | 1:84:A:THR:HB   | 1:87:A:LEU:HB2  | 2                   | 0.14     | 0.02                | 0.14       |
| (1,1823) | 1:84:A:THR:HB   | 1:87:A:LEU:HB3  | 2                   | 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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,893)  | 1:39:A:ILE:HD11 | 1:45:A:TRP:HD1  | 2                   | 0.13     | 0.0                 | 0.13       |
| (1,893)  | 1:39:A:ILE:HD12 | 1:45:A:TRP:HD1  | 2                   | 0.13     | 0.0                 | 0.13       |
| (1,893)  | 1:39:A:ILE:HD13 | 1:45:A:TRP:HD1  | 2                   | 0.13     | 0.0                 | 0.13       |
| (1,1252) | 1:56:A:ASP:HB2  | 1:59:A:ASN:HD21 | 2                   | 0.13     | 0.02                | 0.13       |
| (1,1252) | 1:56:A:ASP:HB2  | 1:59:A:ASN:HD22 | 2                   | 0.13     | 0.02                | 0.13       |
| (1,1252) | 1:56:A:ASP:HB3  | 1:59:A:ASN:HD21 | 2                   | 0.13     | 0.02                | 0.13       |
| (1,1252) | 1:56:A:ASP:HB3  | 1:59:A:ASN:HD22 | 2                   | 0.13     | 0.02                | 0.13       |
| (1,1336) | 1:62:A:TYR:HD1  | 1:63:A:ILE:HG21 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1336) | 1:62:A:TYR:HD1  | 1:63:A:ILE:HG22 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1336) | 1:62:A:TYR:HD1  | 1:63:A:ILE:HG23 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1336) | 1:62:A:TYR:HD2  | 1:63:A:ILE:HG21 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1336) | 1:62:A:TYR:HD2  | 1:63:A:ILE:HG22 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1336) | 1:62:A:TYR:HD2  | 1:63:A:ILE:HG23 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,34)   | 1:3:A:GLU:HG2   | 1:82:A:TYR:HD1  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,34)   | 1:3:A:GLU:HG2   | 1:82:A:TYR:HD2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,34)   | 1:3:A:GLU:HG3   | 1:82:A:TYR:HD1  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,34)   | 1:3:A:GLU:HG3   | 1:82:A:TYR:HD2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,133)  | 1:6:A:THR:HG21  | 1:10:A:ASP:HB2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,133)  | 1:6:A:THR:HG21  | 1:10:A:ASP:HB3  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,133)  | 1:6:A:THR:HG22  | 1:10:A:ASP:HB2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,133)  | 1:6:A:THR:HG22  | 1:10:A:ASP:HB3  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,133)  | 1:6:A:THR:HG23  | 1:10:A:ASP:HB2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,133)  | 1:6:A:THR:HG23  | 1:10:A:ASP:HB3  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,469)  | 1:18:A:GLU:HA   | 1:20:A:LEU:HB2  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,469)  | 1:18:A:GLU:HA   | 1:20:A:LEU:HB3  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,626)  | 1:24:A:LYS:HA   | 1:45:A:TRP:HE1  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,838)  | 1:36:A:SER:HA   | 1:39:A:ILE:HD11 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,838)  | 1:36:A:SER:HA   | 1:39:A:ILE:HD12 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,838)  | 1:36:A:SER:HA   | 1:39:A:ILE:HD13 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1132) | 1:49:A:LEU:HD11 | 1:63:A:ILE:HB   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1132) | 1:49:A:LEU:HD12 | 1:63:A:ILE:HB   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1132) | 1:49:A:LEU:HD13 | 1:63:A:ILE:HB   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1132) | 1:49:A:LEU:HD21 | 1:63:A:ILE:HB   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1132) | 1:49:A:LEU:HD22 | 1:63:A:ILE:HB   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1132) | 1:49:A:LEU:HD23 | 1:63:A:ILE:HB   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,196)  | 1:8:A:LEU:HD11  | 1:11:A:LEU:HB2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,196)  | 1:8:A:LEU:HD11  | 1:11:A:LEU:HB3  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,196)  | 1:8:A:LEU:HD12  | 1:11:A:LEU:HB2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,196)  | 1:8:A:LEU:HD12  | 1:11:A:LEU:HB3  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,196)  | 1:8:A:LEU:HD13  | 1:11:A:LEU:HB2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,196)  | 1:8:A:LEU:HD13  | 1:11:A:LEU:HB3  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,196)  | 1:8:A:LEU:HD21  | 1:11:A:LEU:HB2  | 2                   | 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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,196)  | 1:8:A:LEU:HD21  | 1:11:A:LEU:HB3  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,196)  | 1:8:A:LEU:HD22  | 1:11:A:LEU:HB2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,196)  | 1:8:A:LEU:HD22  | 1:11:A:LEU:HB3  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,196)  | 1:8:A:LEU:HD23  | 1:11:A:LEU:HB2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,196)  | 1:8:A:LEU:HD23  | 1:11:A:LEU:HB3  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,537)  | 1:21:A:GLU:HA   | 1:21:A:GLU:HG2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,537)  | 1:21:A:GLU:HA   | 1:21:A:GLU:HG3  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,803)  | 1:35:A:LYS:HA   | 1:35:A:LYS:HG2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,803)  | 1:35:A:LYS:HA   | 1:35:A:LYS:HG3  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,633)  | 1:25:A:SER:HA   | 1:28:A:LYS:H    | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1346) | 1:62:A:TYR:H    | 1:66:A:ILE:HD11 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1346) | 1:62:A:TYR:H    | 1:66:A:ILE:HD12 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1346) | 1:62:A:TYR:H    | 1:66:A:ILE:HD13 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1608) | 1:73:A:PRO:HA   | 1:73:A:PRO:HD2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1608) | 1:73:A:PRO:HA   | 1:73:A:PRO:HD3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1690) | 1:77:A:THR:HG21 | 1:80:A:VAL:HG11 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1690) | 1:77:A:THR:HG21 | 1:80:A:VAL:HG12 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1690) | 1:77:A:THR:HG21 | 1:80:A:VAL:HG13 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1690) | 1:77:A:THR:HG21 | 1:80:A:VAL:HG21 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1690) | 1:77:A:THR:HG21 | 1:80:A:VAL:HG22 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1690) | 1:77:A:THR:HG21 | 1:80:A:VAL:HG23 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1690) | 1:77:A:THR:HG22 | 1:80:A:VAL:HG11 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1690) | 1:77:A:THR:HG22 | 1:80:A:VAL:HG12 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1690) | 1:77:A:THR:HG22 | 1:80:A:VAL:HG13 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1690) | 1:77:A:THR:HG22 | 1:80:A:VAL:HG21 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1690) | 1:77:A:THR:HG22 | 1:80:A:VAL:HG22 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1690) | 1:77:A:THR:HG22 | 1:80:A:VAL:HG23 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1690) | 1:77:A:THR:HG23 | 1:80:A:VAL:HG11 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1690) | 1:77:A:THR:HG23 | 1:80:A:VAL:HG12 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1690) | 1:77:A:THR:HG23 | 1:80:A:VAL:HG13 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1690) | 1:77:A:THR:HG23 | 1:80:A:VAL:HG21 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1690) | 1:77:A:THR:HG23 | 1:80:A:VAL:HG22 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1690) | 1:77:A:THR:HG23 | 1:80:A:VAL:HG23 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,309)  | 1:11:A:LEU:HD11 | 1:78:A:MET:HB2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,309)  | 1:11:A:LEU:HD11 | 1:78:A:MET:HB3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,309)  | 1:11:A:LEU:HD12 | 1:78:A:MET:HB2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,309)  | 1:11:A:LEU:HD12 | 1:78:A:MET:HB3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,309)  | 1:11:A:LEU:HD13 | 1:78:A:MET:HB2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,309)  | 1:11:A:LEU:HD13 | 1:78:A:MET:HB3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,309)  | 1:11:A:LEU:HD21 | 1:78:A:MET:HB2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,309)  | 1:11:A:LEU:HD21 | 1:78:A:MET:HB3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,309)  | 1:11:A:LEU:HD22 | 1:78:A:MET: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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,309)  | 1:11:A:LEU:HD22 | 1:78:A:MET:HB3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,309)  | 1:11:A:LEU:HD23 | 1:78:A:MET:HB2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,309)  | 1:11:A:LEU:HD23 | 1:78:A:MET:HB3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,839)  | 1:36:A:SER:HB2  | 1:39:A:ILE:HD11 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,839)  | 1:36:A:SER:HB2  | 1:39:A:ILE:HD12 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,839)  | 1:36:A:SER:HB2  | 1:39:A:ILE:HD13 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,839)  | 1:36:A:SER:HB3  | 1:39:A:ILE:HD11 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,839)  | 1:36:A:SER:HB3  | 1:39:A:ILE:HD12 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,839)  | 1:36:A:SER:HB3  | 1:39:A:ILE:HD13 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1128) | 1:49:A:LEU:HD11 | 1:62:A:TYR:HE1  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1128) | 1:49:A:LEU:HD11 | 1:62:A:TYR:HE2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1128) | 1:49:A:LEU:HD12 | 1:62:A:TYR:HE1  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1128) | 1:49:A:LEU:HD12 | 1:62:A:TYR:HE2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1128) | 1:49:A:LEU:HD13 | 1:62:A:TYR:HE1  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1128) | 1:49:A:LEU:HD13 | 1:62:A:TYR:HE2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1128) | 1:49:A:LEU:HD21 | 1:62:A:TYR:HE1  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1128) | 1:49:A:LEU:HD21 | 1:62:A:TYR:HE2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1128) | 1:49:A:LEU:HD22 | 1:62:A:TYR:HE1  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1128) | 1:49:A:LEU:HD22 | 1:62:A:TYR:HE2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1128) | 1:49:A:LEU:HD23 | 1:62:A:TYR:HE1  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1128) | 1:49:A:LEU:HD23 | 1:62:A:TYR:HE2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1241) | 1:56:A:ASP:HB2  | 1:57:A:LYS:H    | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1241) | 1:56:A:ASP:HB3  | 1:57:A:LYS:H    | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1434) | 1:65:A:HIS:HB2  | 1:67:A:PHE:HD1  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1434) | 1:65:A:HIS:HB2  | 1:67:A:PHE:HD2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1434) | 1:65:A:HIS:HB3  | 1:67:A:PHE:HD1  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1434) | 1:65:A:HIS:HB3  | 1:67:A:PHE:HD2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1452) | 1:66:A:ILE:HA   | 1:66:A:ILE:HG12 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1452) | 1:66:A:ILE:HA   | 1:66:A:ILE:HG13 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1461) | 1:66:A:ILE:HG21 | 1:67:A:PHE:HA   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1461) | 1:66:A:ILE:HG22 | 1:67:A:PHE:HA   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1461) | 1:66:A:ILE:HG23 | 1:67:A:PHE:HA   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1547) | 1:69:A:ILE:HB   | 1:69:A:ILE:H    | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,338)  | 1:12:A:THR:HG21 | 1:46:A:PHE:HE1  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,338)  | 1:12:A:THR:HG21 | 1:46:A:PHE:HE2  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,338)  | 1:12:A:THR:HG22 | 1:46:A:PHE:HE1  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,338)  | 1:12:A:THR:HG22 | 1:46:A:PHE:HE2  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,338)  | 1:12:A:THR:HG23 | 1:46:A:PHE:HE1  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,338)  | 1:12:A:THR:HG23 | 1:46:A:PHE:HE2  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,1230) | 1:55:A:LEU:HD11 | 1:60:A:LEU:HA   | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,1230) | 1:55:A:LEU:HD12 | 1:60:A:LEU:HA   | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,1230) | 1:55:A:LEU:HD13 | 1:60:A:LEU:HA   | 2                   | 0.1      | 0.0                 | 0.1        |

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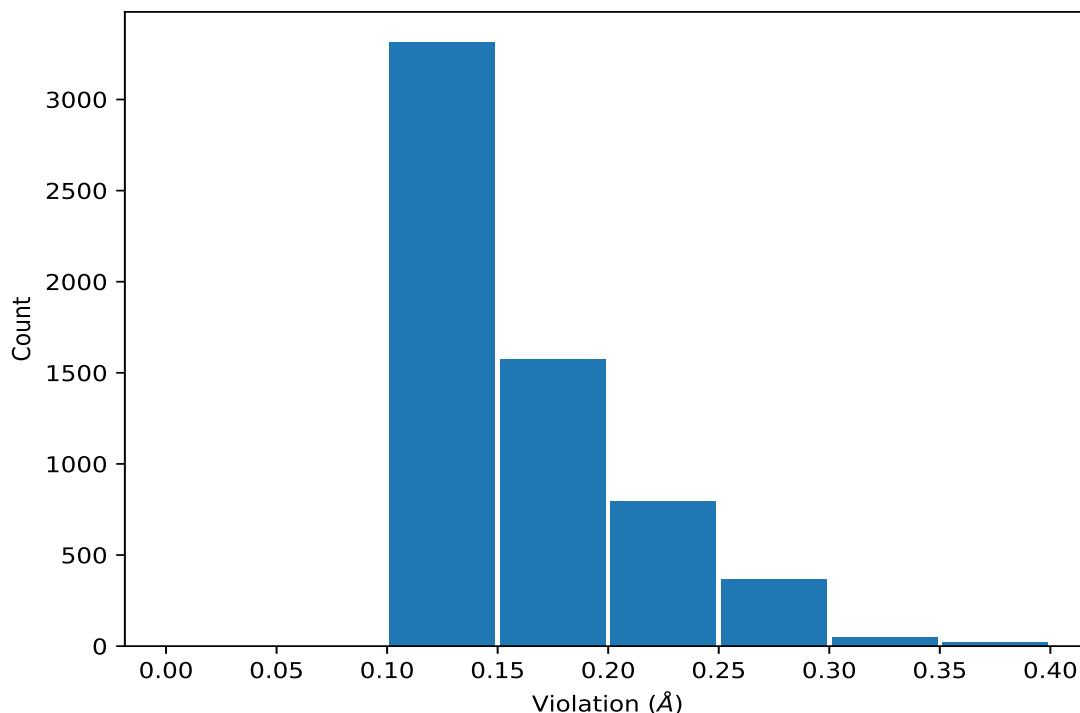
| Key      | Atom-1          | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|---------------|---------------------|----------|---------------------|------------|
| (1,1230) | 1:55:A:LEU:HD21 | 1:60:A:LEU:HA | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,1230) | 1:55:A:LEU:HD22 | 1:60:A:LEU:HA | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,1230) | 1:55:A:LEU:HD23 | 1:60:A:LEU:HA | 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) |
|----------|-----------------|--------------|----------|---------------|
| (1,1462) | 1:66:A:ILE:HG12 | 1:67:A:PHE:H | 13       | 0.39          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1462) | 1:66:A:ILE:HG13 | 1:67:A:PHE:H    | 13       | 0.39          |
| (1,1462) | 1:66:A:ILE:HG12 | 1:67:A:PHE:H    | 16       | 0.39          |
| (1,1462) | 1:66:A:ILE:HG13 | 1:67:A:PHE:H    | 16       | 0.39          |
| (1,1462) | 1:66:A:ILE:HG12 | 1:67:A:PHE:H    | 7        | 0.38          |
| (1,1462) | 1:66:A:ILE:HG13 | 1:67:A:PHE:H    | 7        | 0.38          |
| (1,1273) | 1:58:A:ASP:HA   | 1:59:A:ASN:HD21 | 12       | 0.38          |
| (1,1273) | 1:58:A:ASP:HA   | 1:59:A:ASN:HD22 | 12       | 0.38          |
| (1,1462) | 1:66:A:ILE:HG12 | 1:67:A:PHE:H    | 8        | 0.37          |
| (1,1462) | 1:66:A:ILE:HG13 | 1:67:A:PHE:H    | 8        | 0.37          |
| (1,1462) | 1:66:A:ILE:HG12 | 1:67:A:PHE:H    | 17       | 0.37          |
| (1,1462) | 1:66:A:ILE:HG13 | 1:67:A:PHE:H    | 17       | 0.37          |
| (1,894)  | 1:39:A:ILE:HD11 | 1:45:A:TRP:HH2  | 8        | 0.37          |
| (1,894)  | 1:39:A:ILE:HD12 | 1:45:A:TRP:HH2  | 8        | 0.37          |
| (1,894)  | 1:39:A:ILE:HD13 | 1:45:A:TRP:HH2  | 8        | 0.37          |
| (1,1462) | 1:66:A:ILE:HG12 | 1:67:A:PHE:H    | 4        | 0.36          |
| (1,1462) | 1:66:A:ILE:HG13 | 1:67:A:PHE:H    | 4        | 0.36          |
| (1,1199) | 1:54:A:LYS:HA   | 1:54:A:LYS:HD2  | 10       | 0.36          |
| (1,1199) | 1:54:A:LYS:HA   | 1:54:A:LYS:HD3  | 10       | 0.36          |
| (1,631)  | 1:25:A:SER:H    | 1:27:A:CYS:H    | 20       | 0.36          |
| (1,894)  | 1:39:A:ILE:HD11 | 1:45:A:TRP:HH2  | 7        | 0.35          |
| (1,894)  | 1:39:A:ILE:HD12 | 1:45:A:TRP:HH2  | 7        | 0.35          |
| (1,894)  | 1:39:A:ILE:HD13 | 1:45:A:TRP:HH2  | 7        | 0.35          |
| (1,894)  | 1:39:A:ILE:HD11 | 1:45:A:TRP:HH2  | 15       | 0.35          |
| (1,894)  | 1:39:A:ILE:HD12 | 1:45:A:TRP:HH2  | 15       | 0.35          |
| (1,894)  | 1:39:A:ILE:HD13 | 1:45:A:TRP:HH2  | 15       | 0.35          |
| (1,138)  | 1:7:A:LEU:HA    | 1:7:A:LEU:HG    | 10       | 0.35          |
| (1,1462) | 1:66:A:ILE:HG12 | 1:67:A:PHE:H    | 3        | 0.34          |
| (1,1462) | 1:66:A:ILE:HG13 | 1:67:A:PHE:H    | 3        | 0.34          |
| (1,1462) | 1:66:A:ILE:HG12 | 1:67:A:PHE:H    | 11       | 0.34          |
| (1,1462) | 1:66:A:ILE:HG13 | 1:67:A:PHE:H    | 11       | 0.34          |
| (1,1462) | 1:66:A:ILE:HG12 | 1:67:A:PHE:H    | 18       | 0.33          |
| (1,1462) | 1:66:A:ILE:HG13 | 1:67:A:PHE:H    | 18       | 0.33          |
| (1,1273) | 1:58:A:ASP:HA   | 1:59:A:ASN:HD21 | 4        | 0.33          |
| (1,1273) | 1:58:A:ASP:HA   | 1:59:A:ASN:HD22 | 4        | 0.33          |
| (1,438)  | 1:17:A:LEU:HA   | 1:17:A:LEU:HG   | 1        | 0.33          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD2  | 9        | 0.32          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD3  | 9        | 0.32          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD2  | 9        | 0.32          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD3  | 9        | 0.32          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD2  | 9        | 0.32          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD3  | 9        | 0.32          |
| (1,1462) | 1:66:A:ILE:HG12 | 1:67:A:PHE:H    | 15       | 0.32          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1462) | 1:66:A:ILE:HG13 | 1:67:A:PHE:H    | 15       | 0.32          |
| (1,1199) | 1:54:A:LYS:HA   | 1:54:A:LYS:HD2  | 19       | 0.32          |
| (1,1199) | 1:54:A:LYS:HA   | 1:54:A:LYS:HD3  | 19       | 0.32          |
| (1,631)  | 1:25:A:SER:H    | 1:27:A:CYS:H    | 5        | 0.32          |
| (1,631)  | 1:25:A:SER:H    | 1:27:A:CYS:H    | 8        | 0.32          |
| (1,438)  | 1:17:A:LEU:HA   | 1:17:A:LEU:HG   | 8        | 0.32          |
| (1,138)  | 1:7:A:LEU:HA    | 1:7:A:LEU:HG    | 1        | 0.32          |
| (1,138)  | 1:7:A:LEU:HA    | 1:7:A:LEU:HG    | 14       | 0.32          |
| (1,138)  | 1:7:A:LEU:HA    | 1:7:A:LEU:HG    | 18       | 0.32          |
| (1,1673) | 1:77:A:THR:HG21 | 1:77:A:THR:H    | 19       | 0.31          |
| (1,1673) | 1:77:A:THR:HG22 | 1:77:A:THR:H    | 19       | 0.31          |
| (1,1673) | 1:77:A:THR:HG23 | 1:77:A:THR:H    | 19       | 0.31          |
| (1,1462) | 1:66:A:ILE:HG12 | 1:67:A:PHE:H    | 2        | 0.31          |
| (1,1462) | 1:66:A:ILE:HG13 | 1:67:A:PHE:H    | 2        | 0.31          |
| (1,1462) | 1:66:A:ILE:HG12 | 1:67:A:PHE:H    | 19       | 0.31          |
| (1,1462) | 1:66:A:ILE:HG13 | 1:67:A:PHE:H    | 19       | 0.31          |
| (1,1462) | 1:66:A:ILE:HG12 | 1:67:A:PHE:H    | 20       | 0.31          |
| (1,1462) | 1:66:A:ILE:HG13 | 1:67:A:PHE:H    | 20       | 0.31          |
| (1,631)  | 1:25:A:SER:H    | 1:27:A:CYS:H    | 13       | 0.31          |
| (1,631)  | 1:25:A:SER:H    | 1:27:A:CYS:H    | 16       | 0.31          |
| (1,570)  | 1:22:A:GLN:H    | 1:66:A:ILE:HG21 | 5        | 0.31          |
| (1,570)  | 1:22:A:GLN:H    | 1:66:A:ILE:HG22 | 5        | 0.31          |
| (1,570)  | 1:22:A:GLN:H    | 1:66:A:ILE:HG23 | 5        | 0.31          |
| (1,138)  | 1:7:A:LEU:HA    | 1:7:A:LEU:HG    | 9        | 0.31          |
| (1,138)  | 1:7:A:LEU:HA    | 1:7:A:LEU:HG    | 15       | 0.31          |
| (1,138)  | 1:7:A:LEU:HA    | 1:7:A:LEU:HG    | 16       | 0.31          |
| (1,1879) | 1:88:A:LYS:HD2  | 1:88:A:LYS:HA   | 19       | 0.3           |
| (1,1879) | 1:88:A:LYS:HD3  | 1:88:A:LYS:HA   | 19       | 0.3           |
| (1,1806) | 1:84:A:THR:HG21 | 1:84:A:THR:H    | 2        | 0.3           |
| (1,1806) | 1:84:A:THR:HG22 | 1:84:A:THR:H    | 2        | 0.3           |
| (1,1806) | 1:84:A:THR:HG23 | 1:84:A:THR:H    | 2        | 0.3           |
| (1,1806) | 1:84:A:THR:HG21 | 1:84:A:THR:H    | 10       | 0.3           |
| (1,1806) | 1:84:A:THR:HG22 | 1:84:A:THR:H    | 10       | 0.3           |
| (1,1806) | 1:84:A:THR:HG23 | 1:84:A:THR:H    | 10       | 0.3           |
| (1,1806) | 1:84:A:THR:HG21 | 1:84:A:THR:H    | 11       | 0.3           |
| (1,1806) | 1:84:A:THR:HG22 | 1:84:A:THR:H    | 11       | 0.3           |
| (1,1806) | 1:84:A:THR:HG23 | 1:84:A:THR:H    | 11       | 0.3           |
| (1,1673) | 1:77:A:THR:HG21 | 1:77:A:THR:H    | 3        | 0.3           |
| (1,1673) | 1:77:A:THR:HG22 | 1:77:A:THR:H    | 3        | 0.3           |
| (1,1673) | 1:77:A:THR:HG23 | 1:77:A:THR:H    | 3        | 0.3           |
| (1,1673) | 1:77:A:THR:HG21 | 1:77:A:THR:H    | 13       | 0.3           |
| (1,1673) | 1:77:A:THR:HG22 | 1:77:A:THR:H    | 13       | 0.3           |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1673) | 1:77:A:THR:HG23 | 1:77:A:THR:H   | 13       | 0.3           |
| (1,1673) | 1:77:A:THR:HG21 | 1:77:A:THR:H   | 17       | 0.3           |
| (1,1673) | 1:77:A:THR:HG22 | 1:77:A:THR:H   | 17       | 0.3           |
| (1,1673) | 1:77:A:THR:HG23 | 1:77:A:THR:H   | 17       | 0.3           |
| (1,1462) | 1:66:A:ILE:HG12 | 1:67:A:PHE:H   | 9        | 0.3           |
| (1,1462) | 1:66:A:ILE:HG13 | 1:67:A:PHE:H   | 9        | 0.3           |
| (1,1199) | 1:54:A:LYS:HA   | 1:54:A:LYS:HD2 | 18       | 0.3           |
| (1,1199) | 1:54:A:LYS:HA   | 1:54:A:LYS:HD3 | 18       | 0.3           |
| (1,1129) | 1:49:A:LEU:HG   | 1:62:A:TYR:HD1 | 10       | 0.3           |
| (1,1129) | 1:49:A:LEU:HG   | 1:62:A:TYR:HD2 | 10       | 0.3           |
| (1,918)  | 1:40:A:THR:HA   | 1:41:A:THR:H   | 6        | 0.3           |
| (1,894)  | 1:39:A:ILE:HD11 | 1:45:A:TRP:HH2 | 11       | 0.3           |
| (1,894)  | 1:39:A:ILE:HD12 | 1:45:A:TRP:HH2 | 11       | 0.3           |
| (1,894)  | 1:39:A:ILE:HD13 | 1:45:A:TRP:HH2 | 11       | 0.3           |
| (1,894)  | 1:39:A:ILE:HD11 | 1:45:A:TRP:HH2 | 19       | 0.3           |
| (1,894)  | 1:39:A:ILE:HD12 | 1:45:A:TRP:HH2 | 19       | 0.3           |
| (1,894)  | 1:39:A:ILE:HD13 | 1:45:A:TRP:HH2 | 19       | 0.3           |
| (1,631)  | 1:25:A:SER:H    | 1:27:A:CYS:H   | 1        | 0.3           |
| (1,631)  | 1:25:A:SER:H    | 1:27:A:CYS:H   | 2        | 0.3           |
| (1,631)  | 1:25:A:SER:H    | 1:27:A:CYS:H   | 18       | 0.3           |
| (1,138)  | 1:7:A:LEU:HA    | 1:7:A:LEU:HG   | 4        | 0.3           |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD11 | 14       | 0.3           |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD12 | 14       | 0.3           |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD13 | 14       | 0.3           |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD21 | 14       | 0.3           |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD22 | 14       | 0.3           |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD23 | 14       | 0.3           |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD11 | 14       | 0.3           |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD12 | 14       | 0.3           |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD13 | 14       | 0.3           |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD21 | 14       | 0.3           |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD22 | 14       | 0.3           |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD23 | 14       | 0.3           |
| (1,1806) | 1:84:A:THR:HG21 | 1:84:A:THR:H   | 4        | 0.29          |
| (1,1806) | 1:84:A:THR:HG22 | 1:84:A:THR:H   | 4        | 0.29          |
| (1,1806) | 1:84:A:THR:HG23 | 1:84:A:THR:H   | 4        | 0.29          |
| (1,1806) | 1:84:A:THR:HG21 | 1:84:A:THR:H   | 14       | 0.29          |
| (1,1806) | 1:84:A:THR:HG22 | 1:84:A:THR:H   | 14       | 0.29          |
| (1,1806) | 1:84:A:THR:HG23 | 1:84:A:THR:H   | 14       | 0.29          |
| (1,1806) | 1:84:A:THR:HG21 | 1:84:A:THR:H   | 15       | 0.29          |
| (1,1806) | 1:84:A:THR:HG22 | 1:84:A:THR:H   | 15       | 0.29          |
| (1,1806) | 1:84:A:THR:HG23 | 1:84:A:THR:H   | 15       | 0.29          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1806) | 1:84:A:THR:HG21 | 1:84:A:THR:H   | 19       | 0.29          |
| (1,1806) | 1:84:A:THR:HG22 | 1:84:A:THR:H   | 19       | 0.29          |
| (1,1806) | 1:84:A:THR:HG23 | 1:84:A:THR:H   | 19       | 0.29          |
| (1,1673) | 1:77:A:THR:HG21 | 1:77:A:THR:H   | 7        | 0.29          |
| (1,1673) | 1:77:A:THR:HG22 | 1:77:A:THR:H   | 7        | 0.29          |
| (1,1673) | 1:77:A:THR:HG23 | 1:77:A:THR:H   | 7        | 0.29          |
| (1,1673) | 1:77:A:THR:HG21 | 1:77:A:THR:H   | 8        | 0.29          |
| (1,1673) | 1:77:A:THR:HG22 | 1:77:A:THR:H   | 8        | 0.29          |
| (1,1673) | 1:77:A:THR:HG23 | 1:77:A:THR:H   | 8        | 0.29          |
| (1,1673) | 1:77:A:THR:HG21 | 1:77:A:THR:H   | 10       | 0.29          |
| (1,1673) | 1:77:A:THR:HG22 | 1:77:A:THR:H   | 10       | 0.29          |
| (1,1673) | 1:77:A:THR:HG23 | 1:77:A:THR:H   | 10       | 0.29          |
| (1,1462) | 1:66:A:ILE:HG12 | 1:67:A:PHE:H   | 10       | 0.29          |
| (1,1462) | 1:66:A:ILE:HG13 | 1:67:A:PHE:H   | 10       | 0.29          |
| (1,1462) | 1:66:A:ILE:HG12 | 1:67:A:PHE:H   | 14       | 0.29          |
| (1,1462) | 1:66:A:ILE:HG13 | 1:67:A:PHE:H   | 14       | 0.29          |
| (1,1340) | 1:62:A:TYR:HD1  | 1:63:A:ILE:H   | 3        | 0.29          |
| (1,1340) | 1:62:A:TYR:HD2  | 1:63:A:ILE:H   | 3        | 0.29          |
| (1,1129) | 1:49:A:LEU:HG   | 1:62:A:TYR:HD1 | 1        | 0.29          |
| (1,1129) | 1:49:A:LEU:HG   | 1:62:A:TYR:HD2 | 1        | 0.29          |
| (1,1129) | 1:49:A:LEU:HG   | 1:62:A:TYR:HD1 | 6        | 0.29          |
| (1,1129) | 1:49:A:LEU:HG   | 1:62:A:TYR:HD2 | 6        | 0.29          |
| (1,772)  | 1:31:A:ILE:HG21 | 1:49:A:LEU:HA  | 11       | 0.29          |
| (1,772)  | 1:31:A:ILE:HG22 | 1:49:A:LEU:HA  | 11       | 0.29          |
| (1,772)  | 1:31:A:ILE:HG23 | 1:49:A:LEU:HA  | 11       | 0.29          |
| (1,631)  | 1:25:A:SER:H    | 1:27:A:CYS:H   | 3        | 0.29          |
| (1,631)  | 1:25:A:SER:H    | 1:27:A:CYS:H   | 11       | 0.29          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD11 | 1        | 0.29          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD12 | 1        | 0.29          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD13 | 1        | 0.29          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD21 | 1        | 0.29          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD22 | 1        | 0.29          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD23 | 1        | 0.29          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD11 | 1        | 0.29          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD12 | 1        | 0.29          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD13 | 1        | 0.29          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD21 | 1        | 0.29          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD22 | 1        | 0.29          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD23 | 1        | 0.29          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD11 | 15       | 0.29          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD12 | 15       | 0.29          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD13 | 15       | 0.29          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD21 | 15       | 0.29          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD22 | 15       | 0.29          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD23 | 15       | 0.29          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD11 | 15       | 0.29          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD12 | 15       | 0.29          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD13 | 15       | 0.29          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD21 | 15       | 0.29          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD22 | 15       | 0.29          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD23 | 15       | 0.29          |
| (1,1879) | 1:88:A:LYS:HD2  | 1:88:A:LYS:HA  | 20       | 0.28          |
| (1,1879) | 1:88:A:LYS:HD3  | 1:88:A:LYS:HA  | 20       | 0.28          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD2 | 13       | 0.28          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD3 | 13       | 0.28          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD2 | 13       | 0.28          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD3 | 13       | 0.28          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD2 | 13       | 0.28          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD3 | 13       | 0.28          |
| (1,1806) | 1:84:A:THR:HG21 | 1:84:A:THR:H   | 5        | 0.28          |
| (1,1806) | 1:84:A:THR:HG22 | 1:84:A:THR:H   | 5        | 0.28          |
| (1,1806) | 1:84:A:THR:HG23 | 1:84:A:THR:H   | 5        | 0.28          |
| (1,1806) | 1:84:A:THR:HG21 | 1:84:A:THR:H   | 16       | 0.28          |
| (1,1806) | 1:84:A:THR:HG22 | 1:84:A:THR:H   | 16       | 0.28          |
| (1,1806) | 1:84:A:THR:HG23 | 1:84:A:THR:H   | 16       | 0.28          |
| (1,1806) | 1:84:A:THR:HG21 | 1:84:A:THR:H   | 20       | 0.28          |
| (1,1806) | 1:84:A:THR:HG22 | 1:84:A:THR:H   | 20       | 0.28          |
| (1,1806) | 1:84:A:THR:HG23 | 1:84:A:THR:H   | 20       | 0.28          |
| (1,1673) | 1:77:A:THR:HG21 | 1:77:A:THR:H   | 4        | 0.28          |
| (1,1673) | 1:77:A:THR:HG22 | 1:77:A:THR:H   | 4        | 0.28          |
| (1,1673) | 1:77:A:THR:HG23 | 1:77:A:THR:H   | 4        | 0.28          |
| (1,1673) | 1:77:A:THR:HG21 | 1:77:A:THR:H   | 5        | 0.28          |
| (1,1673) | 1:77:A:THR:HG22 | 1:77:A:THR:H   | 5        | 0.28          |
| (1,1673) | 1:77:A:THR:HG23 | 1:77:A:THR:H   | 5        | 0.28          |
| (1,1673) | 1:77:A:THR:HG21 | 1:77:A:THR:H   | 6        | 0.28          |
| (1,1673) | 1:77:A:THR:HG22 | 1:77:A:THR:H   | 6        | 0.28          |
| (1,1673) | 1:77:A:THR:HG23 | 1:77:A:THR:H   | 6        | 0.28          |
| (1,1673) | 1:77:A:THR:HG21 | 1:77:A:THR:H   | 14       | 0.28          |
| (1,1673) | 1:77:A:THR:HG22 | 1:77:A:THR:H   | 14       | 0.28          |
| (1,1673) | 1:77:A:THR:HG23 | 1:77:A:THR:H   | 14       | 0.28          |
| (1,1673) | 1:77:A:THR:HG21 | 1:77:A:THR:H   | 16       | 0.28          |
| (1,1673) | 1:77:A:THR:HG22 | 1:77:A:THR:H   | 16       | 0.28          |
| (1,1673) | 1:77:A:THR:HG23 | 1:77:A:THR:H   | 16       | 0.28          |
| (1,1673) | 1:77:A:THR:HG21 | 1:77:A:THR:H   | 18       | 0.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1673) | 1:77:A:THR:HG22 | 1:77:A:THR:H    | 18       | 0.28          |
| (1,1673) | 1:77:A:THR:HG23 | 1:77:A:THR:H    | 18       | 0.28          |
| (1,1462) | 1:66:A:ILE:HG12 | 1:67:A:PHE:H    | 1        | 0.28          |
| (1,1462) | 1:66:A:ILE:HG13 | 1:67:A:PHE:H    | 1        | 0.28          |
| (1,1462) | 1:66:A:ILE:HG12 | 1:67:A:PHE:H    | 5        | 0.28          |
| (1,1462) | 1:66:A:ILE:HG13 | 1:67:A:PHE:H    | 5        | 0.28          |
| (1,1462) | 1:66:A:ILE:HG12 | 1:67:A:PHE:H    | 12       | 0.28          |
| (1,1462) | 1:66:A:ILE:HG13 | 1:67:A:PHE:H    | 12       | 0.28          |
| (1,1437) | 1:65:A:HIS:HA   | 1:68:A:GLU:H    | 19       | 0.28          |
| (1,1129) | 1:49:A:LEU:HG   | 1:62:A:TYR:HD1  | 5        | 0.28          |
| (1,1129) | 1:49:A:LEU:HG   | 1:62:A:TYR:HD2  | 5        | 0.28          |
| (1,1129) | 1:49:A:LEU:HG   | 1:62:A:TYR:HD1  | 9        | 0.28          |
| (1,1129) | 1:49:A:LEU:HG   | 1:62:A:TYR:HD2  | 9        | 0.28          |
| (1,1105) | 1:49:A:LEU:HB2  | 1:52:A:HIS:HD2  | 1        | 0.28          |
| (1,1105) | 1:49:A:LEU:HB3  | 1:52:A:HIS:HD2  | 1        | 0.28          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG21 | 9        | 0.28          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG22 | 9        | 0.28          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG23 | 9        | 0.28          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG21 | 9        | 0.28          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG22 | 9        | 0.28          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG23 | 9        | 0.28          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG21 | 9        | 0.28          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG22 | 9        | 0.28          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG23 | 9        | 0.28          |
| (1,631)  | 1:25:A:SER:H    | 1:27:A:CYS:H    | 4        | 0.28          |
| (1,631)  | 1:25:A:SER:H    | 1:27:A:CYS:H    | 7        | 0.28          |
| (1,631)  | 1:25:A:SER:H    | 1:27:A:CYS:H    | 12       | 0.28          |
| (1,631)  | 1:25:A:SER:H    | 1:27:A:CYS:H    | 19       | 0.28          |
| (1,570)  | 1:22:A:GLN:H    | 1:66:A:ILE:HG21 | 10       | 0.28          |
| (1,570)  | 1:22:A:GLN:H    | 1:66:A:ILE:HG22 | 10       | 0.28          |
| (1,570)  | 1:22:A:GLN:H    | 1:66:A:ILE:HG23 | 10       | 0.28          |
| (1,314)  | 1:12:A:THR:HG21 | 1:12:A:THR:H    | 14       | 0.28          |
| (1,314)  | 1:12:A:THR:HG22 | 1:12:A:THR:H    | 14       | 0.28          |
| (1,314)  | 1:12:A:THR:HG23 | 1:12:A:THR:H    | 14       | 0.28          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD11  | 16       | 0.28          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD12  | 16       | 0.28          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD13  | 16       | 0.28          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD21  | 16       | 0.28          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD22  | 16       | 0.28          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD23  | 16       | 0.28          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD11  | 16       | 0.28          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD12  | 16       | 0.28          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD13 | 16       | 0.28          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD21 | 16       | 0.28          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD22 | 16       | 0.28          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD23 | 16       | 0.28          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD2 | 17       | 0.27          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD3 | 17       | 0.27          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD2 | 17       | 0.27          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD3 | 17       | 0.27          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD2 | 17       | 0.27          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD3 | 17       | 0.27          |
| (1,1806) | 1:84:A:THR:HG21 | 1:84:A:THR:H   | 3        | 0.27          |
| (1,1806) | 1:84:A:THR:HG22 | 1:84:A:THR:H   | 3        | 0.27          |
| (1,1806) | 1:84:A:THR:HG23 | 1:84:A:THR:H   | 3        | 0.27          |
| (1,1806) | 1:84:A:THR:HG21 | 1:84:A:THR:H   | 6        | 0.27          |
| (1,1806) | 1:84:A:THR:HG22 | 1:84:A:THR:H   | 6        | 0.27          |
| (1,1806) | 1:84:A:THR:HG23 | 1:84:A:THR:H   | 6        | 0.27          |
| (1,1806) | 1:84:A:THR:HG21 | 1:84:A:THR:H   | 12       | 0.27          |
| (1,1806) | 1:84:A:THR:HG22 | 1:84:A:THR:H   | 12       | 0.27          |
| (1,1806) | 1:84:A:THR:HG23 | 1:84:A:THR:H   | 12       | 0.27          |
| (1,1673) | 1:77:A:THR:HG21 | 1:77:A:THR:H   | 1        | 0.27          |
| (1,1673) | 1:77:A:THR:HG22 | 1:77:A:THR:H   | 1        | 0.27          |
| (1,1673) | 1:77:A:THR:HG23 | 1:77:A:THR:H   | 1        | 0.27          |
| (1,1673) | 1:77:A:THR:HG21 | 1:77:A:THR:H   | 2        | 0.27          |
| (1,1673) | 1:77:A:THR:HG22 | 1:77:A:THR:H   | 2        | 0.27          |
| (1,1673) | 1:77:A:THR:HG23 | 1:77:A:THR:H   | 2        | 0.27          |
| (1,1673) | 1:77:A:THR:HG21 | 1:77:A:THR:H   | 11       | 0.27          |
| (1,1673) | 1:77:A:THR:HG22 | 1:77:A:THR:H   | 11       | 0.27          |
| (1,1673) | 1:77:A:THR:HG23 | 1:77:A:THR:H   | 11       | 0.27          |
| (1,1673) | 1:77:A:THR:HG21 | 1:77:A:THR:H   | 12       | 0.27          |
| (1,1673) | 1:77:A:THR:HG22 | 1:77:A:THR:H   | 12       | 0.27          |
| (1,1673) | 1:77:A:THR:HG23 | 1:77:A:THR:H   | 12       | 0.27          |
| (1,1673) | 1:77:A:THR:HG21 | 1:77:A:THR:H   | 15       | 0.27          |
| (1,1673) | 1:77:A:THR:HG22 | 1:77:A:THR:H   | 15       | 0.27          |
| (1,1673) | 1:77:A:THR:HG23 | 1:77:A:THR:H   | 15       | 0.27          |
| (1,1673) | 1:77:A:THR:HG21 | 1:77:A:THR:H   | 20       | 0.27          |
| (1,1673) | 1:77:A:THR:HG22 | 1:77:A:THR:H   | 20       | 0.27          |
| (1,1673) | 1:77:A:THR:HG23 | 1:77:A:THR:H   | 20       | 0.27          |
| (1,1462) | 1:66:A:ILE:HG12 | 1:67:A:PHE:H   | 6        | 0.27          |
| (1,1462) | 1:66:A:ILE:HG13 | 1:67:A:PHE:H   | 6        | 0.27          |
| (1,1340) | 1:62:A:TYR:HD1  | 1:63:A:ILE:H   | 18       | 0.27          |
| (1,1340) | 1:62:A:TYR:HD2  | 1:63:A:ILE:H   | 18       | 0.27          |
| (1,1129) | 1:49:A:LEU:HG   | 1:62:A:TYR:HD1 | 11       | 0.27          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1129) | 1:49:A:LEU:HG   | 1:62:A:TYR:HD2  | 11       | 0.27          |
| (1,1129) | 1:49:A:LEU:HG   | 1:62:A:TYR:HD1  | 19       | 0.27          |
| (1,1129) | 1:49:A:LEU:HG   | 1:62:A:TYR:HD2  | 19       | 0.27          |
| (1,894)  | 1:39:A:ILE:HD11 | 1:45:A:TRP:HH2  | 13       | 0.27          |
| (1,894)  | 1:39:A:ILE:HD12 | 1:45:A:TRP:HH2  | 13       | 0.27          |
| (1,894)  | 1:39:A:ILE:HD13 | 1:45:A:TRP:HH2  | 13       | 0.27          |
| (1,894)  | 1:39:A:ILE:HD11 | 1:45:A:TRP:HH2  | 16       | 0.27          |
| (1,894)  | 1:39:A:ILE:HD12 | 1:45:A:TRP:HH2  | 16       | 0.27          |
| (1,894)  | 1:39:A:ILE:HD13 | 1:45:A:TRP:HH2  | 16       | 0.27          |
| (1,512)  | 1:20:A:LEU:HB2  | 1:24:A:LYS:HG2  | 11       | 0.27          |
| (1,512)  | 1:20:A:LEU:HB2  | 1:24:A:LYS:HG3  | 11       | 0.27          |
| (1,512)  | 1:20:A:LEU:HB3  | 1:24:A:LYS:HG2  | 11       | 0.27          |
| (1,512)  | 1:20:A:LEU:HB3  | 1:24:A:LYS:HG3  | 11       | 0.27          |
| (1,438)  | 1:17:A:LEU:HA   | 1:17:A:LEU:HG   | 2        | 0.27          |
| (1,438)  | 1:17:A:LEU:HA   | 1:17:A:LEU:HG   | 3        | 0.27          |
| (1,314)  | 1:12:A:THR:HG21 | 1:12:A:THR:H    | 10       | 0.27          |
| (1,314)  | 1:12:A:THR:HG22 | 1:12:A:THR:H    | 10       | 0.27          |
| (1,314)  | 1:12:A:THR:HG23 | 1:12:A:THR:H    | 10       | 0.27          |
| (1,314)  | 1:12:A:THR:HG21 | 1:12:A:THR:H    | 16       | 0.27          |
| (1,314)  | 1:12:A:THR:HG22 | 1:12:A:THR:H    | 16       | 0.27          |
| (1,314)  | 1:12:A:THR:HG23 | 1:12:A:THR:H    | 16       | 0.27          |
| (1,1673) | 1:77:A:THR:HG21 | 1:77:A:THR:H    | 9        | 0.26          |
| (1,1673) | 1:77:A:THR:HG22 | 1:77:A:THR:H    | 9        | 0.26          |
| (1,1673) | 1:77:A:THR:HG23 | 1:77:A:THR:H    | 9        | 0.26          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG11 | 11       | 0.26          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG12 | 11       | 0.26          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG13 | 11       | 0.26          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG21 | 11       | 0.26          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG22 | 11       | 0.26          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG23 | 11       | 0.26          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG11 | 11       | 0.26          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG12 | 11       | 0.26          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG13 | 11       | 0.26          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG21 | 11       | 0.26          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG22 | 11       | 0.26          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG23 | 11       | 0.26          |
| (1,1437) | 1:65:A:HIS:HA   | 1:68:A:GLU:H    | 3        | 0.26          |
| (1,1437) | 1:65:A:HIS:HA   | 1:68:A:GLU:H    | 9        | 0.26          |
| (1,1340) | 1:62:A:TYR:HD1  | 1:63:A:ILE:H    | 8        | 0.26          |
| (1,1340) | 1:62:A:TYR:HD2  | 1:63:A:ILE:H    | 8        | 0.26          |
| (1,1340) | 1:62:A:TYR:HD1  | 1:63:A:ILE:H    | 17       | 0.26          |
| (1,1340) | 1:62:A:TYR:HD2  | 1:63:A:ILE:H    | 17       | 0.26          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1129) | 1:49:A:LEU:HG   | 1:62:A:TYR:HD1 | 12       | 0.26          |
| (1,1129) | 1:49:A:LEU:HG   | 1:62:A:TYR:HD2 | 12       | 0.26          |
| (1,1105) | 1:49:A:LEU:HB2  | 1:52:A:HIS:HD2 | 6        | 0.26          |
| (1,1105) | 1:49:A:LEU:HB3  | 1:52:A:HIS:HD2 | 6        | 0.26          |
| (1,1105) | 1:49:A:LEU:HB2  | 1:52:A:HIS:HD2 | 20       | 0.26          |
| (1,1105) | 1:49:A:LEU:HB3  | 1:52:A:HIS:HD2 | 20       | 0.26          |
| (1,894)  | 1:39:A:ILE:HD11 | 1:45:A:TRP:HH2 | 1        | 0.26          |
| (1,894)  | 1:39:A:ILE:HD12 | 1:45:A:TRP:HH2 | 1        | 0.26          |
| (1,894)  | 1:39:A:ILE:HD13 | 1:45:A:TRP:HH2 | 1        | 0.26          |
| (1,894)  | 1:39:A:ILE:HD11 | 1:45:A:TRP:HH2 | 5        | 0.26          |
| (1,894)  | 1:39:A:ILE:HD12 | 1:45:A:TRP:HH2 | 5        | 0.26          |
| (1,894)  | 1:39:A:ILE:HD13 | 1:45:A:TRP:HH2 | 5        | 0.26          |
| (1,894)  | 1:39:A:ILE:HD11 | 1:45:A:TRP:HH2 | 9        | 0.26          |
| (1,894)  | 1:39:A:ILE:HD12 | 1:45:A:TRP:HH2 | 9        | 0.26          |
| (1,894)  | 1:39:A:ILE:HD13 | 1:45:A:TRP:HH2 | 9        | 0.26          |
| (1,696)  | 1:28:A:LYS:HD2  | 1:29:A:GLU:H   | 3        | 0.26          |
| (1,696)  | 1:28:A:LYS:HD3  | 1:29:A:GLU:H   | 3        | 0.26          |
| (1,631)  | 1:25:A:SER:H    | 1:27:A:CYS:H   | 15       | 0.26          |
| (1,631)  | 1:25:A:SER:H    | 1:27:A:CYS:H   | 17       | 0.26          |
| (1,438)  | 1:17:A:LEU:HA   | 1:17:A:LEU:HG  | 9        | 0.26          |
| (1,438)  | 1:17:A:LEU:HA   | 1:17:A:LEU:HG  | 17       | 0.26          |
| (1,314)  | 1:12:A:THR:HG21 | 1:12:A:THR:H   | 11       | 0.26          |
| (1,314)  | 1:12:A:THR:HG22 | 1:12:A:THR:H   | 11       | 0.26          |
| (1,314)  | 1:12:A:THR:HG23 | 1:12:A:THR:H   | 11       | 0.26          |
| (1,314)  | 1:12:A:THR:HG21 | 1:12:A:THR:H   | 15       | 0.26          |
| (1,314)  | 1:12:A:THR:HG22 | 1:12:A:THR:H   | 15       | 0.26          |
| (1,314)  | 1:12:A:THR:HG23 | 1:12:A:THR:H   | 15       | 0.26          |
| (1,314)  | 1:12:A:THR:HG21 | 1:12:A:THR:H   | 18       | 0.26          |
| (1,314)  | 1:12:A:THR:HG22 | 1:12:A:THR:H   | 18       | 0.26          |
| (1,314)  | 1:12:A:THR:HG23 | 1:12:A:THR:H   | 18       | 0.26          |
| (1,314)  | 1:12:A:THR:HG21 | 1:12:A:THR:H   | 20       | 0.26          |
| (1,314)  | 1:12:A:THR:HG22 | 1:12:A:THR:H   | 20       | 0.26          |
| (1,314)  | 1:12:A:THR:HG23 | 1:12:A:THR:H   | 20       | 0.26          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD11 | 4        | 0.26          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD12 | 4        | 0.26          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD13 | 4        | 0.26          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD21 | 4        | 0.26          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD22 | 4        | 0.26          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD23 | 4        | 0.26          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD11 | 4        | 0.26          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD12 | 4        | 0.26          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD13 | 4        | 0.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD21  | 4        | 0.26          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD22  | 4        | 0.26          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD23  | 4        | 0.26          |
| (1,1273) | 1:58:A:ASP:HA   | 1:59:A:ASN:HD21 | 9        | 0.25          |
| (1,1273) | 1:58:A:ASP:HA   | 1:59:A:ASN:HD22 | 9        | 0.25          |
| (1,1250) | 1:56:A:ASP:H    | 1:59:A:ASN:HB2  | 4        | 0.25          |
| (1,1250) | 1:56:A:ASP:H    | 1:59:A:ASN:HB3  | 4        | 0.25          |
| (1,1199) | 1:54:A:LYS:HA   | 1:54:A:LYS:HD2  | 3        | 0.25          |
| (1,1199) | 1:54:A:LYS:HA   | 1:54:A:LYS:HD3  | 3        | 0.25          |
| (1,1194) | 1:54:A:LYS:HD2  | 1:54:A:LYS:H    | 3        | 0.25          |
| (1,1194) | 1:54:A:LYS:HD3  | 1:54:A:LYS:H    | 3        | 0.25          |
| (1,1194) | 1:54:A:LYS:HD2  | 1:54:A:LYS:H    | 19       | 0.25          |
| (1,1194) | 1:54:A:LYS:HD3  | 1:54:A:LYS:H    | 19       | 0.25          |
| (1,1129) | 1:49:A:LEU:HG   | 1:62:A:TYR:HD1  | 15       | 0.25          |
| (1,1129) | 1:49:A:LEU:HG   | 1:62:A:TYR:HD2  | 15       | 0.25          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG21 | 14       | 0.25          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG22 | 14       | 0.25          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG23 | 14       | 0.25          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG21 | 14       | 0.25          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG22 | 14       | 0.25          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG23 | 14       | 0.25          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG21 | 14       | 0.25          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG22 | 14       | 0.25          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG23 | 14       | 0.25          |
| (1,483)  | 1:19:A:ASP:HA   | 1:22:A:GLN:HE21 | 19       | 0.25          |
| (1,483)  | 1:19:A:ASP:HA   | 1:22:A:GLN:HE22 | 19       | 0.25          |
| (1,314)  | 1:12:A:THR:HG21 | 1:12:A:THR:H    | 1        | 0.25          |
| (1,314)  | 1:12:A:THR:HG22 | 1:12:A:THR:H    | 1        | 0.25          |
| (1,314)  | 1:12:A:THR:HG23 | 1:12:A:THR:H    | 1        | 0.25          |
| (1,314)  | 1:12:A:THR:HG21 | 1:12:A:THR:H    | 2        | 0.25          |
| (1,314)  | 1:12:A:THR:HG22 | 1:12:A:THR:H    | 2        | 0.25          |
| (1,314)  | 1:12:A:THR:HG23 | 1:12:A:THR:H    | 2        | 0.25          |
| (1,314)  | 1:12:A:THR:HG21 | 1:12:A:THR:H    | 5        | 0.25          |
| (1,314)  | 1:12:A:THR:HG22 | 1:12:A:THR:H    | 5        | 0.25          |
| (1,314)  | 1:12:A:THR:HG23 | 1:12:A:THR:H    | 5        | 0.25          |
| (1,314)  | 1:12:A:THR:HG21 | 1:12:A:THR:H    | 7        | 0.25          |
| (1,314)  | 1:12:A:THR:HG22 | 1:12:A:THR:H    | 7        | 0.25          |
| (1,314)  | 1:12:A:THR:HG23 | 1:12:A:THR:H    | 7        | 0.25          |
| (1,314)  | 1:12:A:THR:HG21 | 1:12:A:THR:H    | 8        | 0.25          |
| (1,314)  | 1:12:A:THR:HG22 | 1:12:A:THR:H    | 8        | 0.25          |
| (1,314)  | 1:12:A:THR:HG23 | 1:12:A:THR:H    | 8        | 0.25          |
| (1,314)  | 1:12:A:THR:HG21 | 1:12:A:THR:H    | 17       | 0.25          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,314)  | 1:12:A:THR:HG22 | 1:12:A:THR:H   | 17       | 0.25          |
| (1,314)  | 1:12:A:THR:HG23 | 1:12:A:THR:H   | 17       | 0.25          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD11 | 10       | 0.25          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD12 | 10       | 0.25          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD13 | 10       | 0.25          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD21 | 10       | 0.25          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD22 | 10       | 0.25          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD23 | 10       | 0.25          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD11 | 10       | 0.25          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD12 | 10       | 0.25          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD13 | 10       | 0.25          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD21 | 10       | 0.25          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD22 | 10       | 0.25          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD23 | 10       | 0.25          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD2 | 1        | 0.24          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD3 | 1        | 0.24          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD2 | 1        | 0.24          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD3 | 1        | 0.24          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD2 | 1        | 0.24          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD3 | 1        | 0.24          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD2 | 7        | 0.24          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD3 | 7        | 0.24          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD2 | 7        | 0.24          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD3 | 7        | 0.24          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD2 | 7        | 0.24          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD3 | 7        | 0.24          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD2 | 8        | 0.24          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD3 | 8        | 0.24          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD2 | 8        | 0.24          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD3 | 8        | 0.24          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD2 | 8        | 0.24          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD3 | 8        | 0.24          |
| (1,1806) | 1:84:A:THR:HG21 | 1:84:A:THR:H   | 1        | 0.24          |
| (1,1806) | 1:84:A:THR:HG22 | 1:84:A:THR:H   | 1        | 0.24          |
| (1,1806) | 1:84:A:THR:HG23 | 1:84:A:THR:H   | 1        | 0.24          |
| (1,1806) | 1:84:A:THR:HG21 | 1:84:A:THR:H   | 13       | 0.24          |
| (1,1806) | 1:84:A:THR:HG22 | 1:84:A:THR:H   | 13       | 0.24          |
| (1,1806) | 1:84:A:THR:HG23 | 1:84:A:THR:H   | 13       | 0.24          |
| (1,1806) | 1:84:A:THR:HG21 | 1:84:A:THR:H   | 17       | 0.24          |
| (1,1806) | 1:84:A:THR:HG22 | 1:84:A:THR:H   | 17       | 0.24          |
| (1,1806) | 1:84:A:THR:HG23 | 1:84:A:THR:H   | 17       | 0.24          |
| (1,1806) | 1:84:A:THR:HG21 | 1:84:A:THR:H   | 18       | 0.24          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1806) | 1:84:A:THR:HG22 | 1:84:A:THR:H    | 18       | 0.24          |
| (1,1806) | 1:84:A:THR:HG23 | 1:84:A:THR:H    | 18       | 0.24          |
| (1,1437) | 1:65:A:HIS:HA   | 1:68:A:GLU:H    | 6        | 0.24          |
| (1,1428) | 1:65:A:HIS:HD2  | 1:66:A:ILE:HG12 | 11       | 0.24          |
| (1,1428) | 1:65:A:HIS:HD2  | 1:66:A:ILE:HG13 | 11       | 0.24          |
| (1,1340) | 1:62:A:TYR:HD1  | 1:63:A:ILE:H    | 7        | 0.24          |
| (1,1340) | 1:62:A:TYR:HD2  | 1:63:A:ILE:H    | 7        | 0.24          |
| (1,1200) | 1:54:A:LYS:HA   | 1:54:A:LYS:HE2  | 10       | 0.24          |
| (1,1200) | 1:54:A:LYS:HA   | 1:54:A:LYS:HE3  | 10       | 0.24          |
| (1,1200) | 1:54:A:LYS:HA   | 1:54:A:LYS:HE2  | 18       | 0.24          |
| (1,1200) | 1:54:A:LYS:HA   | 1:54:A:LYS:HE3  | 18       | 0.24          |
| (1,1198) | 1:54:A:LYS:HA   | 1:54:A:LYS:HE2  | 10       | 0.24          |
| (1,1198) | 1:54:A:LYS:HA   | 1:54:A:LYS:HE3  | 10       | 0.24          |
| (1,1198) | 1:54:A:LYS:HA   | 1:54:A:LYS:HE2  | 18       | 0.24          |
| (1,1198) | 1:54:A:LYS:HA   | 1:54:A:LYS:HE3  | 18       | 0.24          |
| (1,1129) | 1:49:A:LEU:HG   | 1:62:A:TYR:HD1  | 2        | 0.24          |
| (1,1129) | 1:49:A:LEU:HG   | 1:62:A:TYR:HD2  | 2        | 0.24          |
| (1,1129) | 1:49:A:LEU:HG   | 1:62:A:TYR:HD1  | 14       | 0.24          |
| (1,1129) | 1:49:A:LEU:HG   | 1:62:A:TYR:HD2  | 14       | 0.24          |
| (1,1105) | 1:49:A:LEU:HB2  | 1:52:A:HIS:HD2  | 14       | 0.24          |
| (1,1105) | 1:49:A:LEU:HB3  | 1:52:A:HIS:HD2  | 14       | 0.24          |
| (1,894)  | 1:39:A:ILE:HD11 | 1:45:A:TRP:HH2  | 3        | 0.24          |
| (1,894)  | 1:39:A:ILE:HD12 | 1:45:A:TRP:HH2  | 3        | 0.24          |
| (1,894)  | 1:39:A:ILE:HD13 | 1:45:A:TRP:HH2  | 3        | 0.24          |
| (1,894)  | 1:39:A:ILE:HD11 | 1:45:A:TRP:HH2  | 12       | 0.24          |
| (1,894)  | 1:39:A:ILE:HD12 | 1:45:A:TRP:HH2  | 12       | 0.24          |
| (1,894)  | 1:39:A:ILE:HD13 | 1:45:A:TRP:HH2  | 12       | 0.24          |
| (1,894)  | 1:39:A:ILE:HD11 | 1:45:A:TRP:HH2  | 14       | 0.24          |
| (1,894)  | 1:39:A:ILE:HD12 | 1:45:A:TRP:HH2  | 14       | 0.24          |
| (1,894)  | 1:39:A:ILE:HD13 | 1:45:A:TRP:HH2  | 14       | 0.24          |
| (1,894)  | 1:39:A:ILE:HD11 | 1:45:A:TRP:HH2  | 17       | 0.24          |
| (1,894)  | 1:39:A:ILE:HD12 | 1:45:A:TRP:HH2  | 17       | 0.24          |
| (1,894)  | 1:39:A:ILE:HD13 | 1:45:A:TRP:HH2  | 17       | 0.24          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG21 | 7        | 0.24          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG22 | 7        | 0.24          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG23 | 7        | 0.24          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG21 | 7        | 0.24          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG22 | 7        | 0.24          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG23 | 7        | 0.24          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG21 | 7        | 0.24          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG22 | 7        | 0.24          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG23 | 7        | 0.24          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,876) | 1:39:A:ILE:HD11 | 1:40:A:THR:HG21 | 15       | 0.24          |
| (1,876) | 1:39:A:ILE:HD11 | 1:40:A:THR:HG22 | 15       | 0.24          |
| (1,876) | 1:39:A:ILE:HD11 | 1:40:A:THR:HG23 | 15       | 0.24          |
| (1,876) | 1:39:A:ILE:HD12 | 1:40:A:THR:HG21 | 15       | 0.24          |
| (1,876) | 1:39:A:ILE:HD12 | 1:40:A:THR:HG22 | 15       | 0.24          |
| (1,876) | 1:39:A:ILE:HD12 | 1:40:A:THR:HG23 | 15       | 0.24          |
| (1,876) | 1:39:A:ILE:HD13 | 1:40:A:THR:HG21 | 15       | 0.24          |
| (1,876) | 1:39:A:ILE:HD13 | 1:40:A:THR:HG22 | 15       | 0.24          |
| (1,876) | 1:39:A:ILE:HD13 | 1:40:A:THR:HG23 | 15       | 0.24          |
| (1,743) | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD2  | 2        | 0.24          |
| (1,743) | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD3  | 2        | 0.24          |
| (1,743) | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD2  | 2        | 0.24          |
| (1,743) | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD3  | 2        | 0.24          |
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD2  | 2        | 0.24          |
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD3  | 2        | 0.24          |
| (1,631) | 1:25:A:SER:H    | 1:27:A:CYS:H    | 6        | 0.24          |
| (1,631) | 1:25:A:SER:H    | 1:27:A:CYS:H    | 9        | 0.24          |
| (1,631) | 1:25:A:SER:H    | 1:27:A:CYS:H    | 14       | 0.24          |
| (1,627) | 1:24:A:LYS:HG2  | 1:45:A:TRP:HD1  | 8        | 0.24          |
| (1,627) | 1:24:A:LYS:HG3  | 1:45:A:TRP:HD1  | 8        | 0.24          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG21 | 2        | 0.24          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG22 | 2        | 0.24          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG23 | 2        | 0.24          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB2  | 1        | 0.24          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB3  | 1        | 0.24          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB2  | 1        | 0.24          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB3  | 1        | 0.24          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB2  | 1        | 0.24          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB3  | 1        | 0.24          |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE1  | 15       | 0.24          |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE2  | 15       | 0.24          |
| (1,314) | 1:12:A:THR:HG21 | 1:12:A:THR:H    | 6        | 0.24          |
| (1,314) | 1:12:A:THR:HG22 | 1:12:A:THR:H    | 6        | 0.24          |
| (1,314) | 1:12:A:THR:HG23 | 1:12:A:THR:H    | 6        | 0.24          |
| (1,314) | 1:12:A:THR:HG21 | 1:12:A:THR:H    | 9        | 0.24          |
| (1,314) | 1:12:A:THR:HG22 | 1:12:A:THR:H    | 9        | 0.24          |
| (1,314) | 1:12:A:THR:HG23 | 1:12:A:THR:H    | 9        | 0.24          |
| (1,314) | 1:12:A:THR:HG21 | 1:12:A:THR:H    | 12       | 0.24          |
| (1,314) | 1:12:A:THR:HG22 | 1:12:A:THR:H    | 12       | 0.24          |
| (1,314) | 1:12:A:THR:HG23 | 1:12:A:THR:H    | 12       | 0.24          |
| (1,314) | 1:12:A:THR:HG21 | 1:12:A:THR:H    | 13       | 0.24          |
| (1,314) | 1:12:A:THR:HG22 | 1:12:A:THR:H    | 13       | 0.24          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,314) | 1:12:A:THR:HG23 | 1:12:A:THR:H    | 13       | 0.24          |
| (1,314) | 1:12:A:THR:HG21 | 1:12:A:THR:H    | 19       | 0.24          |
| (1,314) | 1:12:A:THR:HG22 | 1:12:A:THR:H    | 19       | 0.24          |
| (1,314) | 1:12:A:THR:HG23 | 1:12:A:THR:H    | 19       | 0.24          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD11 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD12 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD13 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD21 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD22 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD23 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD11 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD12 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD13 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD21 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD22 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD23 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD11 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD12 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD13 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD21 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD22 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD23 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD11 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD12 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD13 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD21 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD22 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD23 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD11 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD12 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD13 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD21 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD22 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD23 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD11 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD12 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD13 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD21 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD22 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD23 | 7        | 0.24          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD11 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD12 | 12       | 0.24          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD13 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD21 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD22 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD23 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD11 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD12 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD13 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD21 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD22 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD23 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD11 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD12 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD13 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD21 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD22 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD23 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD11 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD12 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD13 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD21 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD22 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD23 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD11 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD12 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD13 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD21 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD22 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD23 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD11 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD12 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD13 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD21 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD22 | 12       | 0.24          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD23 | 12       | 0.24          |
| (1,67)  | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD11  | 9        | 0.24          |
| (1,67)  | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD12  | 9        | 0.24          |
| (1,67)  | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD13  | 9        | 0.24          |
| (1,67)  | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD21  | 9        | 0.24          |
| (1,67)  | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD22  | 9        | 0.24          |
| (1,67)  | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD23  | 9        | 0.24          |
| (1,67)  | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD11  | 9        | 0.24          |
| (1,67)  | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD12  | 9        | 0.24          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD13  | 9        | 0.24          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD21  | 9        | 0.24          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD22  | 9        | 0.24          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD23  | 9        | 0.24          |
| (1,1806) | 1:84:A:THR:HG21 | 1:84:A:THR:H    | 7        | 0.23          |
| (1,1806) | 1:84:A:THR:HG22 | 1:84:A:THR:H    | 7        | 0.23          |
| (1,1806) | 1:84:A:THR:HG23 | 1:84:A:THR:H    | 7        | 0.23          |
| (1,1669) | 1:76:A:LEU:HD11 | 1:80:A:VAL:HB   | 19       | 0.23          |
| (1,1669) | 1:76:A:LEU:HD12 | 1:80:A:VAL:HB   | 19       | 0.23          |
| (1,1669) | 1:76:A:LEU:HD13 | 1:80:A:VAL:HB   | 19       | 0.23          |
| (1,1669) | 1:76:A:LEU:HD21 | 1:80:A:VAL:HB   | 19       | 0.23          |
| (1,1669) | 1:76:A:LEU:HD22 | 1:80:A:VAL:HB   | 19       | 0.23          |
| (1,1669) | 1:76:A:LEU:HD23 | 1:80:A:VAL:HB   | 19       | 0.23          |
| (1,1550) | 1:69:A:ILE:HA   | 1:69:A:ILE:HD11 | 6        | 0.23          |
| (1,1550) | 1:69:A:ILE:HA   | 1:69:A:ILE:HD12 | 6        | 0.23          |
| (1,1550) | 1:69:A:ILE:HA   | 1:69:A:ILE:HD13 | 6        | 0.23          |
| (1,1340) | 1:62:A:TYR:HD1  | 1:63:A:ILE:H    | 13       | 0.23          |
| (1,1340) | 1:62:A:TYR:HD2  | 1:63:A:ILE:H    | 13       | 0.23          |
| (1,1250) | 1:56:A:ASP:H    | 1:59:A:ASN:HB2  | 19       | 0.23          |
| (1,1250) | 1:56:A:ASP:H    | 1:59:A:ASN:HB3  | 19       | 0.23          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG21 | 18       | 0.23          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG22 | 18       | 0.23          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG23 | 18       | 0.23          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG21 | 18       | 0.23          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG22 | 18       | 0.23          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG23 | 18       | 0.23          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG21 | 18       | 0.23          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG22 | 18       | 0.23          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG23 | 18       | 0.23          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG21 | 19       | 0.23          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG22 | 19       | 0.23          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG23 | 19       | 0.23          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG21 | 19       | 0.23          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG22 | 19       | 0.23          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG23 | 19       | 0.23          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG21 | 19       | 0.23          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG22 | 19       | 0.23          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG23 | 19       | 0.23          |
| (1,772)  | 1:31:A:ILE:HG21 | 1:49:A:LEU:HA   | 7        | 0.23          |
| (1,772)  | 1:31:A:ILE:HG22 | 1:49:A:LEU:HA   | 7        | 0.23          |
| (1,772)  | 1:31:A:ILE:HG23 | 1:49:A:LEU:HA   | 7        | 0.23          |
| (1,631)  | 1:25:A:SER:H    | 1:27:A:CYS:H    | 10       | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,627)  | 1:24:A:LYS:HG2  | 1:45:A:TRP:HD1  | 5        | 0.23          |
| (1,627)  | 1:24:A:LYS:HG3  | 1:45:A:TRP:HD1  | 5        | 0.23          |
| (1,570)  | 1:22:A:GLN:H    | 1:66:A:ILE:HG21 | 1        | 0.23          |
| (1,570)  | 1:22:A:GLN:H    | 1:66:A:ILE:HG22 | 1        | 0.23          |
| (1,570)  | 1:22:A:GLN:H    | 1:66:A:ILE:HG23 | 1        | 0.23          |
| (1,570)  | 1:22:A:GLN:H    | 1:66:A:ILE:HG21 | 3        | 0.23          |
| (1,570)  | 1:22:A:GLN:H    | 1:66:A:ILE:HG22 | 3        | 0.23          |
| (1,570)  | 1:22:A:GLN:H    | 1:66:A:ILE:HG23 | 3        | 0.23          |
| (1,570)  | 1:22:A:GLN:H    | 1:66:A:ILE:HG21 | 11       | 0.23          |
| (1,570)  | 1:22:A:GLN:H    | 1:66:A:ILE:HG22 | 11       | 0.23          |
| (1,570)  | 1:22:A:GLN:H    | 1:66:A:ILE:HG23 | 11       | 0.23          |
| (1,438)  | 1:17:A:LEU:HA   | 1:17:A:LEU:HG   | 5        | 0.23          |
| (1,425)  | 1:16:A:THR:HG21 | 1:18:A:GLU:H    | 12       | 0.23          |
| (1,425)  | 1:16:A:THR:HG22 | 1:18:A:GLU:H    | 12       | 0.23          |
| (1,425)  | 1:16:A:THR:HG23 | 1:18:A:GLU:H    | 12       | 0.23          |
| (1,314)  | 1:12:A:THR:HG21 | 1:12:A:THR:H    | 4        | 0.23          |
| (1,314)  | 1:12:A:THR:HG22 | 1:12:A:THR:H    | 4        | 0.23          |
| (1,314)  | 1:12:A:THR:HG23 | 1:12:A:THR:H    | 4        | 0.23          |
| (1,93)   | 1:4:A:TYR:HA    | 1:82:A:TYR:HE1  | 1        | 0.23          |
| (1,93)   | 1:4:A:TYR:HA    | 1:82:A:TYR:HE2  | 1        | 0.23          |
| (1,1825) | 1:84:A:THR:HB   | 1:87:A:LEU:HG   | 13       | 0.22          |
| (1,1806) | 1:84:A:THR:HG21 | 1:84:A:THR:H    | 8        | 0.22          |
| (1,1806) | 1:84:A:THR:HG22 | 1:84:A:THR:H    | 8        | 0.22          |
| (1,1806) | 1:84:A:THR:HG23 | 1:84:A:THR:H    | 8        | 0.22          |
| (1,1806) | 1:84:A:THR:HG21 | 1:84:A:THR:H    | 9        | 0.22          |
| (1,1806) | 1:84:A:THR:HG22 | 1:84:A:THR:H    | 9        | 0.22          |
| (1,1806) | 1:84:A:THR:HG23 | 1:84:A:THR:H    | 9        | 0.22          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG11 | 13       | 0.22          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG12 | 13       | 0.22          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG13 | 13       | 0.22          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG21 | 13       | 0.22          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG22 | 13       | 0.22          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG23 | 13       | 0.22          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG11 | 13       | 0.22          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG12 | 13       | 0.22          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG13 | 13       | 0.22          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG21 | 13       | 0.22          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG22 | 13       | 0.22          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG23 | 13       | 0.22          |
| (1,1550) | 1:69:A:ILE:HA   | 1:69:A:ILE:HD11 | 4        | 0.22          |
| (1,1550) | 1:69:A:ILE:HA   | 1:69:A:ILE:HD12 | 4        | 0.22          |
| (1,1550) | 1:69:A:ILE:HA   | 1:69:A:ILE:HD13 | 4        | 0.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1550) | 1:69:A:ILE:HA   | 1:69:A:ILE:HD11 | 12       | 0.22          |
| (1,1550) | 1:69:A:ILE:HA   | 1:69:A:ILE:HD12 | 12       | 0.22          |
| (1,1550) | 1:69:A:ILE:HA   | 1:69:A:ILE:HD13 | 12       | 0.22          |
| (1,1550) | 1:69:A:ILE:HA   | 1:69:A:ILE:HD11 | 13       | 0.22          |
| (1,1550) | 1:69:A:ILE:HA   | 1:69:A:ILE:HD12 | 13       | 0.22          |
| (1,1550) | 1:69:A:ILE:HA   | 1:69:A:ILE:HD13 | 13       | 0.22          |
| (1,1550) | 1:69:A:ILE:HA   | 1:69:A:ILE:HD11 | 17       | 0.22          |
| (1,1550) | 1:69:A:ILE:HA   | 1:69:A:ILE:HD12 | 17       | 0.22          |
| (1,1550) | 1:69:A:ILE:HA   | 1:69:A:ILE:HD13 | 17       | 0.22          |
| (1,1437) | 1:65:A:HIS:HA   | 1:68:A:GLU:H    | 12       | 0.22          |
| (1,1437) | 1:65:A:HIS:HA   | 1:68:A:GLU:H    | 14       | 0.22          |
| (1,1428) | 1:65:A:HIS:HD2  | 1:66:A:ILE:HG12 | 16       | 0.22          |
| (1,1428) | 1:65:A:HIS:HD2  | 1:66:A:ILE:HG13 | 16       | 0.22          |
| (1,1357) | 1:63:A:ILE:HA   | 1:63:A:ILE:HD11 | 8        | 0.22          |
| (1,1357) | 1:63:A:ILE:HA   | 1:63:A:ILE:HD12 | 8        | 0.22          |
| (1,1357) | 1:63:A:ILE:HA   | 1:63:A:ILE:HD13 | 8        | 0.22          |
| (1,1357) | 1:63:A:ILE:HA   | 1:63:A:ILE:HD11 | 13       | 0.22          |
| (1,1357) | 1:63:A:ILE:HA   | 1:63:A:ILE:HD12 | 13       | 0.22          |
| (1,1357) | 1:63:A:ILE:HA   | 1:63:A:ILE:HD13 | 13       | 0.22          |
| (1,1351) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HG12 | 2        | 0.22          |
| (1,1351) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HG13 | 2        | 0.22          |
| (1,1351) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HG12 | 2        | 0.22          |
| (1,1351) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HG13 | 2        | 0.22          |
| (1,1351) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HG12 | 8        | 0.22          |
| (1,1351) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HG13 | 8        | 0.22          |
| (1,1351) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HG12 | 8        | 0.22          |
| (1,1351) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HG13 | 8        | 0.22          |
| (1,1340) | 1:62:A:TYR:HD1  | 1:63:A:ILE:H    | 4        | 0.22          |
| (1,1340) | 1:62:A:TYR:HD2  | 1:63:A:ILE:H    | 4        | 0.22          |
| (1,1340) | 1:62:A:TYR:HD1  | 1:63:A:ILE:H    | 16       | 0.22          |
| (1,1340) | 1:62:A:TYR:HD2  | 1:63:A:ILE:H    | 16       | 0.22          |
| (1,1313) | 1:61:A:SER:H    | 1:62:A:TYR:H    | 8        | 0.22          |
| (1,1251) | 1:56:A:ASP:H    | 1:59:A:ASN:HD21 | 12       | 0.22          |
| (1,1251) | 1:56:A:ASP:H    | 1:59:A:ASN:HD22 | 12       | 0.22          |
| (1,1194) | 1:54:A:LYS:HD2  | 1:54:A:LYS:H    | 18       | 0.22          |
| (1,1194) | 1:54:A:LYS:HD3  | 1:54:A:LYS:H    | 18       | 0.22          |
| (1,1105) | 1:49:A:LEU:HB2  | 1:52:A:HIS:HD2  | 11       | 0.22          |
| (1,1105) | 1:49:A:LEU:HB3  | 1:52:A:HIS:HD2  | 11       | 0.22          |
| (1,918)  | 1:40:A:THR:HA   | 1:41:A:THR:H    | 16       | 0.22          |
| (1,894)  | 1:39:A:ILE:HD11 | 1:45:A:TRP:HH2  | 6        | 0.22          |
| (1,894)  | 1:39:A:ILE:HD12 | 1:45:A:TRP:HH2  | 6        | 0.22          |
| (1,894)  | 1:39:A:ILE:HD13 | 1:45:A:TRP:HH2  | 6        | 0.22          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,876) | 1:39:A:ILE:HD11 | 1:40:A:THR:HG21 | 12       | 0.22          |
| (1,876) | 1:39:A:ILE:HD11 | 1:40:A:THR:HG22 | 12       | 0.22          |
| (1,876) | 1:39:A:ILE:HD11 | 1:40:A:THR:HG23 | 12       | 0.22          |
| (1,876) | 1:39:A:ILE:HD12 | 1:40:A:THR:HG21 | 12       | 0.22          |
| (1,876) | 1:39:A:ILE:HD12 | 1:40:A:THR:HG22 | 12       | 0.22          |
| (1,876) | 1:39:A:ILE:HD12 | 1:40:A:THR:HG23 | 12       | 0.22          |
| (1,876) | 1:39:A:ILE:HD13 | 1:40:A:THR:HG21 | 12       | 0.22          |
| (1,876) | 1:39:A:ILE:HD13 | 1:40:A:THR:HG22 | 12       | 0.22          |
| (1,876) | 1:39:A:ILE:HD13 | 1:40:A:THR:HG23 | 12       | 0.22          |
| (1,846) | 1:37:A:GLU:HA   | 1:38:A:GLU:H    | 1        | 0.22          |
| (1,846) | 1:37:A:GLU:HA   | 1:38:A:GLU:H    | 8        | 0.22          |
| (1,772) | 1:31:A:ILE:HG21 | 1:49:A:LEU:HA   | 18       | 0.22          |
| (1,772) | 1:31:A:ILE:HG22 | 1:49:A:LEU:HA   | 18       | 0.22          |
| (1,772) | 1:31:A:ILE:HG23 | 1:49:A:LEU:HA   | 18       | 0.22          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG21 | 6        | 0.22          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG22 | 6        | 0.22          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG23 | 6        | 0.22          |
| (1,512) | 1:20:A:LEU:HB2  | 1:24:A:LYS:HG2  | 12       | 0.22          |
| (1,512) | 1:20:A:LEU:HB2  | 1:24:A:LYS:HG3  | 12       | 0.22          |
| (1,512) | 1:20:A:LEU:HB3  | 1:24:A:LYS:HG2  | 12       | 0.22          |
| (1,512) | 1:20:A:LEU:HB3  | 1:24:A:LYS:HG3  | 12       | 0.22          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB2  | 2        | 0.22          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB3  | 2        | 0.22          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB2  | 2        | 0.22          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB3  | 2        | 0.22          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB2  | 2        | 0.22          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB3  | 2        | 0.22          |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE1  | 3        | 0.22          |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE2  | 3        | 0.22          |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE1  | 7        | 0.22          |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE2  | 7        | 0.22          |
| (1,314) | 1:12:A:THR:HG21 | 1:12:A:THR:H    | 3        | 0.22          |
| (1,314) | 1:12:A:THR:HG22 | 1:12:A:THR:H    | 3        | 0.22          |
| (1,314) | 1:12:A:THR:HG23 | 1:12:A:THR:H    | 3        | 0.22          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD11 | 11       | 0.22          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD12 | 11       | 0.22          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD13 | 11       | 0.22          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD21 | 11       | 0.22          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD22 | 11       | 0.22          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD23 | 11       | 0.22          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD11 | 11       | 0.22          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD12 | 11       | 0.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,296)  | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD13 | 11       | 0.22          |
| (1,296)  | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD21 | 11       | 0.22          |
| (1,296)  | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD22 | 11       | 0.22          |
| (1,296)  | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD23 | 11       | 0.22          |
| (1,296)  | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD11 | 11       | 0.22          |
| (1,296)  | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD12 | 11       | 0.22          |
| (1,296)  | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD13 | 11       | 0.22          |
| (1,296)  | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD21 | 11       | 0.22          |
| (1,296)  | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD22 | 11       | 0.22          |
| (1,296)  | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD23 | 11       | 0.22          |
| (1,296)  | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD11 | 11       | 0.22          |
| (1,296)  | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD12 | 11       | 0.22          |
| (1,296)  | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD13 | 11       | 0.22          |
| (1,296)  | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD21 | 11       | 0.22          |
| (1,296)  | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD22 | 11       | 0.22          |
| (1,296)  | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD23 | 11       | 0.22          |
| (1,296)  | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD11 | 11       | 0.22          |
| (1,296)  | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD12 | 11       | 0.22          |
| (1,296)  | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD13 | 11       | 0.22          |
| (1,296)  | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD21 | 11       | 0.22          |
| (1,296)  | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD22 | 11       | 0.22          |
| (1,296)  | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD23 | 11       | 0.22          |
| (1,296)  | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD11 | 11       | 0.22          |
| (1,296)  | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD12 | 11       | 0.22          |
| (1,296)  | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD13 | 11       | 0.22          |
| (1,296)  | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD21 | 11       | 0.22          |
| (1,296)  | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD22 | 11       | 0.22          |
| (1,296)  | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD23 | 11       | 0.22          |
| (1,10)   | 1:1:A:MET:HA    | 1:57:A:LYS:HD2  | 6        | 0.22          |
| (1,10)   | 1:1:A:MET:HA    | 1:57:A:LYS:HD3  | 6        | 0.22          |
| (1,1825) | 1:84:A:THR:HB   | 1:87:A:LEU:HG   | 2        | 0.21          |
| (1,1825) | 1:84:A:THR:HB   | 1:87:A:LEU:HG   | 17       | 0.21          |
| (1,1825) | 1:84:A:THR:HB   | 1:87:A:LEU:HG   | 19       | 0.21          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD2  | 6        | 0.21          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD3  | 6        | 0.21          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD2  | 6        | 0.21          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD3  | 6        | 0.21          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD2  | 6        | 0.21          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD3  | 6        | 0.21          |
| (1,1550) | 1:69:A:ILE:HA   | 1:69:A:ILE:HD11 | 7        | 0.21          |
| (1,1550) | 1:69:A:ILE:HA   | 1:69:A:ILE:HD12 | 7        | 0.21          |
| (1,1550) | 1:69:A:ILE:HA   | 1:69:A:ILE:HD13 | 7        | 0.21          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD11 | 8        | 0.21          |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD12 | 8        | 0.21          |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD13 | 8        | 0.21          |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD11 | 9        | 0.21          |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD12 | 9        | 0.21          |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD13 | 9        | 0.21          |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD11 | 20       | 0.21          |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD12 | 20       | 0.21          |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD13 | 20       | 0.21          |
| (1,1437) | 1:65:A:HIS:HA  | 1:68:A:GLU:H    | 10       | 0.21          |
| (1,1437) | 1:65:A:HIS:HA  | 1:68:A:GLU:H    | 18       | 0.21          |
| (1,1428) | 1:65:A:HIS:HD2 | 1:66:A:ILE:HG12 | 7        | 0.21          |
| (1,1428) | 1:65:A:HIS:HD2 | 1:66:A:ILE:HG13 | 7        | 0.21          |
| (1,1428) | 1:65:A:HIS:HD2 | 1:66:A:ILE:HG12 | 13       | 0.21          |
| (1,1428) | 1:65:A:HIS:HD2 | 1:66:A:ILE:HG13 | 13       | 0.21          |
| (1,1428) | 1:65:A:HIS:HD2 | 1:66:A:ILE:HG12 | 15       | 0.21          |
| (1,1428) | 1:65:A:HIS:HD2 | 1:66:A:ILE:HG13 | 15       | 0.21          |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG12 | 3        | 0.21          |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG13 | 3        | 0.21          |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG12 | 3        | 0.21          |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG13 | 3        | 0.21          |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG12 | 7        | 0.21          |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG13 | 7        | 0.21          |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG12 | 7        | 0.21          |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG13 | 7        | 0.21          |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG12 | 15       | 0.21          |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG13 | 15       | 0.21          |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG12 | 15       | 0.21          |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG13 | 15       | 0.21          |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG12 | 19       | 0.21          |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG13 | 19       | 0.21          |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG12 | 19       | 0.21          |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG13 | 19       | 0.21          |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG12 | 20       | 0.21          |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG13 | 20       | 0.21          |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG12 | 20       | 0.21          |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG13 | 20       | 0.21          |
| (1,1273) | 1:58:A:ASP:HA  | 1:59:A:ASN:HD21 | 2        | 0.21          |
| (1,1273) | 1:58:A:ASP:HA  | 1:59:A:ASN:HD22 | 2        | 0.21          |
| (1,1194) | 1:54:A:LYS:HD2 | 1:54:A:LYS:H    | 10       | 0.21          |
| (1,1194) | 1:54:A:LYS:HD3 | 1:54:A:LYS:H    | 10       | 0.21          |
| (1,1129) | 1:49:A:LEU:HG  | 1:62:A:TYR:HD1  | 20       | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1129) | 1:49:A:LEU:HG   | 1:62:A:TYR:HD2  | 20       | 0.21          |
| (1,1105) | 1:49:A:LEU:HB2  | 1:52:A:HIS:HD2  | 4        | 0.21          |
| (1,1105) | 1:49:A:LEU:HB3  | 1:52:A:HIS:HD2  | 4        | 0.21          |
| (1,1105) | 1:49:A:LEU:HB2  | 1:52:A:HIS:HD2  | 12       | 0.21          |
| (1,1105) | 1:49:A:LEU:HB3  | 1:52:A:HIS:HD2  | 12       | 0.21          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG21 | 17       | 0.21          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG22 | 17       | 0.21          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG23 | 17       | 0.21          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG21 | 17       | 0.21          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG22 | 17       | 0.21          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG23 | 17       | 0.21          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG21 | 17       | 0.21          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG22 | 17       | 0.21          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG23 | 17       | 0.21          |
| (1,855)  | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD11 | 1        | 0.21          |
| (1,855)  | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD12 | 1        | 0.21          |
| (1,855)  | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD13 | 1        | 0.21          |
| (1,855)  | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD11 | 1        | 0.21          |
| (1,855)  | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD12 | 1        | 0.21          |
| (1,855)  | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD13 | 1        | 0.21          |
| (1,855)  | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD11 | 5        | 0.21          |
| (1,855)  | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD12 | 5        | 0.21          |
| (1,855)  | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD13 | 5        | 0.21          |
| (1,855)  | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD11 | 5        | 0.21          |
| (1,855)  | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD12 | 5        | 0.21          |
| (1,855)  | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD13 | 5        | 0.21          |
| (1,855)  | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD11 | 11       | 0.21          |
| (1,855)  | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD12 | 11       | 0.21          |
| (1,855)  | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD13 | 11       | 0.21          |
| (1,855)  | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD11 | 11       | 0.21          |
| (1,855)  | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD12 | 11       | 0.21          |
| (1,855)  | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD13 | 11       | 0.21          |
| (1,772)  | 1:31:A:ILE:HG21 | 1:49:A:LEU:HA   | 14       | 0.21          |
| (1,772)  | 1:31:A:ILE:HG22 | 1:49:A:LEU:HA   | 14       | 0.21          |
| (1,772)  | 1:31:A:ILE:HG23 | 1:49:A:LEU:HA   | 14       | 0.21          |
| (1,772)  | 1:31:A:ILE:HG21 | 1:49:A:LEU:HA   | 16       | 0.21          |
| (1,772)  | 1:31:A:ILE:HG22 | 1:49:A:LEU:HA   | 16       | 0.21          |
| (1,772)  | 1:31:A:ILE:HG23 | 1:49:A:LEU:HA   | 16       | 0.21          |
| (1,743)  | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD2  | 15       | 0.21          |
| (1,743)  | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD3  | 15       | 0.21          |
| (1,743)  | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD2  | 15       | 0.21          |
| (1,743)  | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD3  | 15       | 0.21          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD2  | 15       | 0.21          |
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD3  | 15       | 0.21          |
| (1,627) | 1:24:A:LYS:HG2  | 1:45:A:TRP:HD1  | 1        | 0.21          |
| (1,627) | 1:24:A:LYS:HG3  | 1:45:A:TRP:HD1  | 1        | 0.21          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG21 | 12       | 0.21          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG22 | 12       | 0.21          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG23 | 12       | 0.21          |
| (1,566) | 1:22:A:GLN:HG2  | 1:25:A:SER:HB2  | 6        | 0.21          |
| (1,566) | 1:22:A:GLN:HG2  | 1:25:A:SER:HB3  | 6        | 0.21          |
| (1,566) | 1:22:A:GLN:HG3  | 1:25:A:SER:HB2  | 6        | 0.21          |
| (1,566) | 1:22:A:GLN:HG3  | 1:25:A:SER:HB3  | 6        | 0.21          |
| (1,512) | 1:20:A:LEU:HB2  | 1:24:A:LYS:HG2  | 9        | 0.21          |
| (1,512) | 1:20:A:LEU:HB2  | 1:24:A:LYS:HG3  | 9        | 0.21          |
| (1,512) | 1:20:A:LEU:HB3  | 1:24:A:LYS:HG2  | 9        | 0.21          |
| (1,512) | 1:20:A:LEU:HB3  | 1:24:A:LYS:HG3  | 9        | 0.21          |
| (1,512) | 1:20:A:LEU:HB2  | 1:24:A:LYS:HG2  | 15       | 0.21          |
| (1,512) | 1:20:A:LEU:HB2  | 1:24:A:LYS:HG3  | 15       | 0.21          |
| (1,512) | 1:20:A:LEU:HB3  | 1:24:A:LYS:HG2  | 15       | 0.21          |
| (1,512) | 1:20:A:LEU:HB3  | 1:24:A:LYS:HG3  | 15       | 0.21          |
| (1,512) | 1:20:A:LEU:HB2  | 1:24:A:LYS:HG2  | 16       | 0.21          |
| (1,512) | 1:20:A:LEU:HB2  | 1:24:A:LYS:HG3  | 16       | 0.21          |
| (1,512) | 1:20:A:LEU:HB3  | 1:24:A:LYS:HG2  | 16       | 0.21          |
| (1,512) | 1:20:A:LEU:HB3  | 1:24:A:LYS:HG3  | 16       | 0.21          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB2  | 13       | 0.21          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB3  | 13       | 0.21          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB2  | 13       | 0.21          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB3  | 13       | 0.21          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB2  | 13       | 0.21          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB3  | 13       | 0.21          |
| (1,420) | 1:16:A:THR:HG21 | 1:17:A:LEU:H    | 15       | 0.21          |
| (1,420) | 1:16:A:THR:HG22 | 1:17:A:LEU:H    | 15       | 0.21          |
| (1,420) | 1:16:A:THR:HG23 | 1:17:A:LEU:H    | 15       | 0.21          |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE1  | 6        | 0.21          |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE2  | 6        | 0.21          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD11 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD12 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD13 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD21 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD22 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD23 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD11 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD12 | 10       | 0.21          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD13 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD21 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD22 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD23 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD11 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD12 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD13 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD21 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD22 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD23 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD11 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD12 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD13 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD21 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD22 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD23 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD11 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD12 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD13 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD21 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD22 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD23 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD11 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD12 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD13 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD21 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD22 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD23 | 10       | 0.21          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD11 | 19       | 0.21          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD12 | 19       | 0.21          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD13 | 19       | 0.21          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD21 | 19       | 0.21          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD22 | 19       | 0.21          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD23 | 19       | 0.21          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD11 | 19       | 0.21          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD12 | 19       | 0.21          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD13 | 19       | 0.21          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD21 | 19       | 0.21          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD22 | 19       | 0.21          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD23 | 19       | 0.21          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD11 | 19       | 0.21          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD12 | 19       | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,296)  | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD13 | 19       | 0.21          |
| (1,296)  | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD21 | 19       | 0.21          |
| (1,296)  | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD22 | 19       | 0.21          |
| (1,296)  | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD23 | 19       | 0.21          |
| (1,296)  | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD11 | 19       | 0.21          |
| (1,296)  | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD12 | 19       | 0.21          |
| (1,296)  | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD13 | 19       | 0.21          |
| (1,296)  | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD21 | 19       | 0.21          |
| (1,296)  | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD22 | 19       | 0.21          |
| (1,296)  | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD23 | 19       | 0.21          |
| (1,296)  | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD11 | 19       | 0.21          |
| (1,296)  | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD12 | 19       | 0.21          |
| (1,296)  | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD13 | 19       | 0.21          |
| (1,296)  | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD21 | 19       | 0.21          |
| (1,296)  | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD22 | 19       | 0.21          |
| (1,296)  | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD23 | 19       | 0.21          |
| (1,296)  | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD11 | 19       | 0.21          |
| (1,296)  | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD12 | 19       | 0.21          |
| (1,296)  | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD13 | 19       | 0.21          |
| (1,296)  | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD21 | 19       | 0.21          |
| (1,296)  | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD22 | 19       | 0.21          |
| (1,296)  | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD23 | 19       | 0.21          |
| (1,112)  | 1:6:A:THR:HG21  | 1:6:A:THR:H     | 1        | 0.21          |
| (1,112)  | 1:6:A:THR:HG22  | 1:6:A:THR:H     | 1        | 0.21          |
| (1,112)  | 1:6:A:THR:HG23  | 1:6:A:THR:H     | 1        | 0.21          |
| (1,112)  | 1:6:A:THR:HG21  | 1:6:A:THR:H     | 13       | 0.21          |
| (1,112)  | 1:6:A:THR:HG22  | 1:6:A:THR:H     | 13       | 0.21          |
| (1,112)  | 1:6:A:THR:HG23  | 1:6:A:THR:H     | 13       | 0.21          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD11  | 18       | 0.21          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD12  | 18       | 0.21          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD13  | 18       | 0.21          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD21  | 18       | 0.21          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD22  | 18       | 0.21          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD23  | 18       | 0.21          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD11  | 18       | 0.21          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD12  | 18       | 0.21          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD13  | 18       | 0.21          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD21  | 18       | 0.21          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD22  | 18       | 0.21          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD23  | 18       | 0.21          |
| (1,1879) | 1:88:A:LYS:HD2  | 1:88:A:LYS:HA   | 15       | 0.2           |
| (1,1879) | 1:88:A:LYS:HD3  | 1:88:A:LYS:HA   | 15       | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1794) | 1:83:A:ARG:HG2  | 1:84:A:THR:H    | 6        | 0.2           |
| (1,1794) | 1:83:A:ARG:HG3  | 1:84:A:THR:H    | 6        | 0.2           |
| (1,1777) | 1:82:A:TYR:HD1  | 1:85:A:ARG:HG2  | 16       | 0.2           |
| (1,1777) | 1:82:A:TYR:HD1  | 1:85:A:ARG:HG3  | 16       | 0.2           |
| (1,1777) | 1:82:A:TYR:HD2  | 1:85:A:ARG:HG2  | 16       | 0.2           |
| (1,1777) | 1:82:A:TYR:HD2  | 1:85:A:ARG:HG3  | 16       | 0.2           |
| (1,1762) | 1:82:A:TYR:HE1  | 1:82:A:TYR:H    | 11       | 0.2           |
| (1,1762) | 1:82:A:TYR:HE2  | 1:82:A:TYR:H    | 11       | 0.2           |
| (1,1669) | 1:76:A:LEU:HD11 | 1:80:A:VAL:HB   | 18       | 0.2           |
| (1,1669) | 1:76:A:LEU:HD12 | 1:80:A:VAL:HB   | 18       | 0.2           |
| (1,1669) | 1:76:A:LEU:HD13 | 1:80:A:VAL:HB   | 18       | 0.2           |
| (1,1669) | 1:76:A:LEU:HD21 | 1:80:A:VAL:HB   | 18       | 0.2           |
| (1,1669) | 1:76:A:LEU:HD22 | 1:80:A:VAL:HB   | 18       | 0.2           |
| (1,1669) | 1:76:A:LEU:HD23 | 1:80:A:VAL:HB   | 18       | 0.2           |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG11 | 4        | 0.2           |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG12 | 4        | 0.2           |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG13 | 4        | 0.2           |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG21 | 4        | 0.2           |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG22 | 4        | 0.2           |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG23 | 4        | 0.2           |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG11 | 4        | 0.2           |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG12 | 4        | 0.2           |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG13 | 4        | 0.2           |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG21 | 4        | 0.2           |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG22 | 4        | 0.2           |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG23 | 4        | 0.2           |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG11 | 9        | 0.2           |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG12 | 9        | 0.2           |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG13 | 9        | 0.2           |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG21 | 9        | 0.2           |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG22 | 9        | 0.2           |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG23 | 9        | 0.2           |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG11 | 9        | 0.2           |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG12 | 9        | 0.2           |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG13 | 9        | 0.2           |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG21 | 9        | 0.2           |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG22 | 9        | 0.2           |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG23 | 9        | 0.2           |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG11 | 18       | 0.2           |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG12 | 18       | 0.2           |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG13 | 18       | 0.2           |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG21 | 18       | 0.2           |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG22 | 18       | 0.2           |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG23 | 18       | 0.2           |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG11 | 18       | 0.2           |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG12 | 18       | 0.2           |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG13 | 18       | 0.2           |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG21 | 18       | 0.2           |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG22 | 18       | 0.2           |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG23 | 18       | 0.2           |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD11 | 2        | 0.2           |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD12 | 2        | 0.2           |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD13 | 2        | 0.2           |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD11 | 3        | 0.2           |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD12 | 3        | 0.2           |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD13 | 3        | 0.2           |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD11 | 5        | 0.2           |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD12 | 5        | 0.2           |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD13 | 5        | 0.2           |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD11 | 18       | 0.2           |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD12 | 18       | 0.2           |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD13 | 18       | 0.2           |
| (1,1454) | 1:66:A:ILE:HA  | 1:67:A:PHE:H    | 19       | 0.2           |
| (1,1428) | 1:65:A:HIS:HD2 | 1:66:A:ILE:HG12 | 17       | 0.2           |
| (1,1428) | 1:65:A:HIS:HD2 | 1:66:A:ILE:HG13 | 17       | 0.2           |
| (1,1428) | 1:65:A:HIS:HD2 | 1:66:A:ILE:HG12 | 19       | 0.2           |
| (1,1428) | 1:65:A:HIS:HD2 | 1:66:A:ILE:HG13 | 19       | 0.2           |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD11 | 4        | 0.2           |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD12 | 4        | 0.2           |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD13 | 4        | 0.2           |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD11 | 14       | 0.2           |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD12 | 14       | 0.2           |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD13 | 14       | 0.2           |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG12 | 5        | 0.2           |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG13 | 5        | 0.2           |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG12 | 5        | 0.2           |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG13 | 5        | 0.2           |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG12 | 14       | 0.2           |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG13 | 14       | 0.2           |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG12 | 14       | 0.2           |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG13 | 14       | 0.2           |
| (1,1273) | 1:58:A:ASP:HA  | 1:59:A:ASN:HD21 | 1        | 0.2           |
| (1,1273) | 1:58:A:ASP:HA  | 1:59:A:ASN:HD22 | 1        | 0.2           |
| (1,1273) | 1:58:A:ASP:HA  | 1:59:A:ASN:HD21 | 7        | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1273) | 1:58:A:ASP:HA   | 1:59:A:ASN:HD22 | 7        | 0.2           |
| (1,1273) | 1:58:A:ASP:HA   | 1:59:A:ASN:HD21 | 19       | 0.2           |
| (1,1273) | 1:58:A:ASP:HA   | 1:59:A:ASN:HD22 | 19       | 0.2           |
| (1,1259) | 1:57:A:LYS:HE2  | 1:58:A:ASP:H    | 20       | 0.2           |
| (1,1259) | 1:57:A:LYS:HE3  | 1:58:A:ASP:H    | 20       | 0.2           |
| (1,1211) | 1:54:A:LYS:HB2  | 1:62:A:TYR:H    | 7        | 0.2           |
| (1,1211) | 1:54:A:LYS:HB3  | 1:62:A:TYR:H    | 7        | 0.2           |
| (1,1200) | 1:54:A:LYS:HA   | 1:54:A:LYS:HE2  | 3        | 0.2           |
| (1,1200) | 1:54:A:LYS:HA   | 1:54:A:LYS:HE3  | 3        | 0.2           |
| (1,1198) | 1:54:A:LYS:HA   | 1:54:A:LYS:HE2  | 3        | 0.2           |
| (1,1198) | 1:54:A:LYS:HA   | 1:54:A:LYS:HE3  | 3        | 0.2           |
| (1,1105) | 1:49:A:LEU:HB2  | 1:52:A:HIS:HD2  | 3        | 0.2           |
| (1,1105) | 1:49:A:LEU:HB3  | 1:52:A:HIS:HD2  | 3        | 0.2           |
| (1,1105) | 1:49:A:LEU:HB2  | 1:52:A:HIS:HD2  | 5        | 0.2           |
| (1,1105) | 1:49:A:LEU:HB3  | 1:52:A:HIS:HD2  | 5        | 0.2           |
| (1,1105) | 1:49:A:LEU:HB2  | 1:52:A:HIS:HD2  | 16       | 0.2           |
| (1,1105) | 1:49:A:LEU:HB3  | 1:52:A:HIS:HD2  | 16       | 0.2           |
| (1,894)  | 1:39:A:ILE:HD11 | 1:45:A:TRP:HH2  | 2        | 0.2           |
| (1,894)  | 1:39:A:ILE:HD12 | 1:45:A:TRP:HH2  | 2        | 0.2           |
| (1,894)  | 1:39:A:ILE:HD13 | 1:45:A:TRP:HH2  | 2        | 0.2           |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG21 | 3        | 0.2           |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG22 | 3        | 0.2           |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG23 | 3        | 0.2           |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG21 | 3        | 0.2           |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG22 | 3        | 0.2           |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG23 | 3        | 0.2           |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG21 | 3        | 0.2           |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG22 | 3        | 0.2           |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG23 | 3        | 0.2           |
| (1,855)  | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD11 | 2        | 0.2           |
| (1,855)  | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD12 | 2        | 0.2           |
| (1,855)  | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD13 | 2        | 0.2           |
| (1,855)  | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD11 | 2        | 0.2           |
| (1,855)  | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD12 | 2        | 0.2           |
| (1,855)  | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD13 | 2        | 0.2           |
| (1,846)  | 1:37:A:GLU:HA   | 1:38:A:GLU:H    | 5        | 0.2           |
| (1,846)  | 1:37:A:GLU:HA   | 1:38:A:GLU:H    | 7        | 0.2           |
| (1,844)  | 1:37:A:GLU:H    | 1:38:A:GLU:H    | 2        | 0.2           |
| (1,844)  | 1:37:A:GLU:H    | 1:38:A:GLU:H    | 10       | 0.2           |
| (1,844)  | 1:37:A:GLU:H    | 1:38:A:GLU:H    | 12       | 0.2           |
| (1,772)  | 1:31:A:ILE:HG21 | 1:49:A:LEU:HA   | 10       | 0.2           |
| (1,772)  | 1:31:A:ILE:HG22 | 1:49:A:LEU:HA   | 10       | 0.2           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,772) | 1:31:A:ILE:HG23 | 1:49:A:LEU:HA   | 10       | 0.2           |
| (1,743) | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD2  | 13       | 0.2           |
| (1,743) | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD3  | 13       | 0.2           |
| (1,743) | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD2  | 13       | 0.2           |
| (1,743) | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD3  | 13       | 0.2           |
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD2  | 13       | 0.2           |
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD3  | 13       | 0.2           |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG21 | 9        | 0.2           |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG22 | 9        | 0.2           |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG23 | 9        | 0.2           |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG21 | 18       | 0.2           |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG22 | 18       | 0.2           |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG23 | 18       | 0.2           |
| (1,512) | 1:20:A:LEU:HB2  | 1:24:A:LYS:HG2  | 14       | 0.2           |
| (1,512) | 1:20:A:LEU:HB2  | 1:24:A:LYS:HG3  | 14       | 0.2           |
| (1,512) | 1:20:A:LEU:HB3  | 1:24:A:LYS:HG2  | 14       | 0.2           |
| (1,512) | 1:20:A:LEU:HB3  | 1:24:A:LYS:HG3  | 14       | 0.2           |
| (1,512) | 1:20:A:LEU:HB2  | 1:24:A:LYS:HG2  | 19       | 0.2           |
| (1,512) | 1:20:A:LEU:HB2  | 1:24:A:LYS:HG3  | 19       | 0.2           |
| (1,512) | 1:20:A:LEU:HB3  | 1:24:A:LYS:HG2  | 19       | 0.2           |
| (1,512) | 1:20:A:LEU:HB3  | 1:24:A:LYS:HG3  | 19       | 0.2           |
| (1,483) | 1:19:A:ASP:HA   | 1:22:A:GLN:HE21 | 9        | 0.2           |
| (1,483) | 1:19:A:ASP:HA   | 1:22:A:GLN:HE22 | 9        | 0.2           |
| (1,425) | 1:16:A:THR:HG21 | 1:18:A:GLU:H    | 14       | 0.2           |
| (1,425) | 1:16:A:THR:HG22 | 1:18:A:GLU:H    | 14       | 0.2           |
| (1,425) | 1:16:A:THR:HG23 | 1:18:A:GLU:H    | 14       | 0.2           |
| (1,420) | 1:16:A:THR:HG21 | 1:17:A:LEU:H    | 12       | 0.2           |
| (1,420) | 1:16:A:THR:HG22 | 1:17:A:LEU:H    | 12       | 0.2           |
| (1,420) | 1:16:A:THR:HG23 | 1:17:A:LEU:H    | 12       | 0.2           |
| (1,420) | 1:16:A:THR:HG21 | 1:17:A:LEU:H    | 20       | 0.2           |
| (1,420) | 1:16:A:THR:HG22 | 1:17:A:LEU:H    | 20       | 0.2           |
| (1,420) | 1:16:A:THR:HG23 | 1:17:A:LEU:H    | 20       | 0.2           |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE1  | 8        | 0.2           |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE2  | 8        | 0.2           |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE1  | 9        | 0.2           |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE2  | 9        | 0.2           |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE1  | 11       | 0.2           |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE2  | 11       | 0.2           |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE1  | 12       | 0.2           |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE2  | 12       | 0.2           |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE1  | 14       | 0.2           |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE2  | 14       | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,341)  | 1:12:A:THR:H    | 1:46:A:PHE:HE1  | 18       | 0.2           |
| (1,341)  | 1:12:A:THR:H    | 1:46:A:PHE:HE2  | 18       | 0.2           |
| (1,341)  | 1:12:A:THR:H    | 1:46:A:PHE:HE1  | 20       | 0.2           |
| (1,341)  | 1:12:A:THR:H    | 1:46:A:PHE:HE2  | 20       | 0.2           |
| (1,232)  | 1:9:A:GLN:HA    | 1:9:A:GLN:HG2   | 10       | 0.2           |
| (1,232)  | 1:9:A:GLN:HA    | 1:9:A:GLN:HG3   | 10       | 0.2           |
| (1,112)  | 1:6:A:THR:HG21  | 1:6:A:THR:H     | 5        | 0.2           |
| (1,112)  | 1:6:A:THR:HG22  | 1:6:A:THR:H     | 5        | 0.2           |
| (1,112)  | 1:6:A:THR:HG23  | 1:6:A:THR:H     | 5        | 0.2           |
| (1,112)  | 1:6:A:THR:HG21  | 1:6:A:THR:H     | 15       | 0.2           |
| (1,112)  | 1:6:A:THR:HG22  | 1:6:A:THR:H     | 15       | 0.2           |
| (1,112)  | 1:6:A:THR:HG23  | 1:6:A:THR:H     | 15       | 0.2           |
| (1,1825) | 1:84:A:THR:HB   | 1:87:A:LEU:HG   | 5        | 0.19          |
| (1,1825) | 1:84:A:THR:HB   | 1:87:A:LEU:HG   | 6        | 0.19          |
| (1,1796) | 1:83:A:ARG:HD2  | 1:84:A:THR:HG21 | 9        | 0.19          |
| (1,1796) | 1:83:A:ARG:HD2  | 1:84:A:THR:HG22 | 9        | 0.19          |
| (1,1796) | 1:83:A:ARG:HD2  | 1:84:A:THR:HG23 | 9        | 0.19          |
| (1,1796) | 1:83:A:ARG:HD3  | 1:84:A:THR:HG21 | 9        | 0.19          |
| (1,1796) | 1:83:A:ARG:HD3  | 1:84:A:THR:HG22 | 9        | 0.19          |
| (1,1796) | 1:83:A:ARG:HD3  | 1:84:A:THR:HG23 | 9        | 0.19          |
| (1,1777) | 1:82:A:TYR:HD1  | 1:85:A:ARG:HG2  | 15       | 0.19          |
| (1,1777) | 1:82:A:TYR:HD1  | 1:85:A:ARG:HG3  | 15       | 0.19          |
| (1,1777) | 1:82:A:TYR:HD2  | 1:85:A:ARG:HG2  | 15       | 0.19          |
| (1,1777) | 1:82:A:TYR:HD2  | 1:85:A:ARG:HG3  | 15       | 0.19          |
| (1,1669) | 1:76:A:LEU:HD11 | 1:80:A:VAL:HB   | 12       | 0.19          |
| (1,1669) | 1:76:A:LEU:HD12 | 1:80:A:VAL:HB   | 12       | 0.19          |
| (1,1669) | 1:76:A:LEU:HD13 | 1:80:A:VAL:HB   | 12       | 0.19          |
| (1,1669) | 1:76:A:LEU:HD21 | 1:80:A:VAL:HB   | 12       | 0.19          |
| (1,1669) | 1:76:A:LEU:HD22 | 1:80:A:VAL:HB   | 12       | 0.19          |
| (1,1669) | 1:76:A:LEU:HD23 | 1:80:A:VAL:HB   | 12       | 0.19          |
| (1,1669) | 1:76:A:LEU:HD11 | 1:80:A:VAL:HB   | 14       | 0.19          |
| (1,1669) | 1:76:A:LEU:HD12 | 1:80:A:VAL:HB   | 14       | 0.19          |
| (1,1669) | 1:76:A:LEU:HD13 | 1:80:A:VAL:HB   | 14       | 0.19          |
| (1,1669) | 1:76:A:LEU:HD21 | 1:80:A:VAL:HB   | 14       | 0.19          |
| (1,1669) | 1:76:A:LEU:HD22 | 1:80:A:VAL:HB   | 14       | 0.19          |
| (1,1669) | 1:76:A:LEU:HD23 | 1:80:A:VAL:HB   | 14       | 0.19          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG11 | 2        | 0.19          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG12 | 2        | 0.19          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG13 | 2        | 0.19          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG21 | 2        | 0.19          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG22 | 2        | 0.19          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG23 | 2        | 0.19          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG11 | 2        | 0.19          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG12 | 2        | 0.19          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG13 | 2        | 0.19          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG21 | 2        | 0.19          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG22 | 2        | 0.19          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG23 | 2        | 0.19          |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG11 | 17       | 0.19          |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG12 | 17       | 0.19          |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG13 | 17       | 0.19          |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG21 | 17       | 0.19          |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG22 | 17       | 0.19          |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG23 | 17       | 0.19          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG11 | 17       | 0.19          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG12 | 17       | 0.19          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG13 | 17       | 0.19          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG21 | 17       | 0.19          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG22 | 17       | 0.19          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG23 | 17       | 0.19          |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG11 | 20       | 0.19          |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG12 | 20       | 0.19          |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG13 | 20       | 0.19          |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG21 | 20       | 0.19          |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG22 | 20       | 0.19          |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG23 | 20       | 0.19          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG11 | 20       | 0.19          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG12 | 20       | 0.19          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG13 | 20       | 0.19          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG21 | 20       | 0.19          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG22 | 20       | 0.19          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG23 | 20       | 0.19          |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD11 | 1        | 0.19          |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD12 | 1        | 0.19          |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD13 | 1        | 0.19          |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD11 | 10       | 0.19          |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD12 | 10       | 0.19          |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD13 | 10       | 0.19          |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD11 | 14       | 0.19          |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD12 | 14       | 0.19          |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD13 | 14       | 0.19          |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD11 | 15       | 0.19          |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD12 | 15       | 0.19          |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD13 | 15       | 0.19          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD11 | 16       | 0.19          |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD12 | 16       | 0.19          |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD13 | 16       | 0.19          |
| (1,1541) | 1:68:A:GLU:HG2 | 1:76:A:LEU:HD11 | 12       | 0.19          |
| (1,1541) | 1:68:A:GLU:HG2 | 1:76:A:LEU:HD12 | 12       | 0.19          |
| (1,1541) | 1:68:A:GLU:HG2 | 1:76:A:LEU:HD13 | 12       | 0.19          |
| (1,1541) | 1:68:A:GLU:HG2 | 1:76:A:LEU:HD21 | 12       | 0.19          |
| (1,1541) | 1:68:A:GLU:HG2 | 1:76:A:LEU:HD22 | 12       | 0.19          |
| (1,1541) | 1:68:A:GLU:HG2 | 1:76:A:LEU:HD23 | 12       | 0.19          |
| (1,1541) | 1:68:A:GLU:HG3 | 1:76:A:LEU:HD11 | 12       | 0.19          |
| (1,1541) | 1:68:A:GLU:HG3 | 1:76:A:LEU:HD12 | 12       | 0.19          |
| (1,1541) | 1:68:A:GLU:HG3 | 1:76:A:LEU:HD13 | 12       | 0.19          |
| (1,1541) | 1:68:A:GLU:HG3 | 1:76:A:LEU:HD21 | 12       | 0.19          |
| (1,1541) | 1:68:A:GLU:HG3 | 1:76:A:LEU:HD22 | 12       | 0.19          |
| (1,1541) | 1:68:A:GLU:HG3 | 1:76:A:LEU:HD23 | 12       | 0.19          |
| (1,1437) | 1:65:A:HIS:HA  | 1:68:A:GLU:H    | 4        | 0.19          |
| (1,1437) | 1:65:A:HIS:HA  | 1:68:A:GLU:H    | 8        | 0.19          |
| (1,1428) | 1:65:A:HIS:HD2 | 1:66:A:ILE:HG12 | 20       | 0.19          |
| (1,1428) | 1:65:A:HIS:HD2 | 1:66:A:ILE:HG13 | 20       | 0.19          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD11 | 1        | 0.19          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD12 | 1        | 0.19          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD13 | 1        | 0.19          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD11 | 2        | 0.19          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD12 | 2        | 0.19          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD13 | 2        | 0.19          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD11 | 3        | 0.19          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD12 | 3        | 0.19          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD13 | 3        | 0.19          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD11 | 7        | 0.19          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD12 | 7        | 0.19          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD13 | 7        | 0.19          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD11 | 15       | 0.19          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD12 | 15       | 0.19          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD13 | 15       | 0.19          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD11 | 16       | 0.19          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD12 | 16       | 0.19          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD13 | 16       | 0.19          |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG12 | 4        | 0.19          |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG13 | 4        | 0.19          |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG12 | 4        | 0.19          |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG13 | 4        | 0.19          |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG12 | 9        | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1351) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HG13 | 9        | 0.19          |
| (1,1351) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HG12 | 9        | 0.19          |
| (1,1351) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HG13 | 9        | 0.19          |
| (1,1351) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HG12 | 12       | 0.19          |
| (1,1351) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HG13 | 12       | 0.19          |
| (1,1351) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HG12 | 12       | 0.19          |
| (1,1351) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HG13 | 12       | 0.19          |
| (1,1351) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HG12 | 13       | 0.19          |
| (1,1351) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HG13 | 13       | 0.19          |
| (1,1351) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HG12 | 13       | 0.19          |
| (1,1351) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HG13 | 13       | 0.19          |
| (1,1273) | 1:58:A:ASP:HA   | 1:59:A:ASN:HD21 | 13       | 0.19          |
| (1,1273) | 1:58:A:ASP:HA   | 1:59:A:ASN:HD22 | 13       | 0.19          |
| (1,1273) | 1:58:A:ASP:HA   | 1:59:A:ASN:HD21 | 16       | 0.19          |
| (1,1273) | 1:58:A:ASP:HA   | 1:59:A:ASN:HD22 | 16       | 0.19          |
| (1,1256) | 1:57:A:LYS:HA   | 1:57:A:LYS:HD2  | 7        | 0.19          |
| (1,1256) | 1:57:A:LYS:HA   | 1:57:A:LYS:HD3  | 7        | 0.19          |
| (1,1228) | 1:55:A:LEU:HG   | 1:59:A:ASN:HD21 | 10       | 0.19          |
| (1,1228) | 1:55:A:LEU:HG   | 1:59:A:ASN:HD22 | 10       | 0.19          |
| (1,1228) | 1:55:A:LEU:HG   | 1:59:A:ASN:HD21 | 13       | 0.19          |
| (1,1228) | 1:55:A:LEU:HG   | 1:59:A:ASN:HD22 | 13       | 0.19          |
| (1,1223) | 1:55:A:LEU:HG   | 1:56:A:ASP:HA   | 8        | 0.19          |
| (1,1200) | 1:54:A:LYS:HA   | 1:54:A:LYS:HE2  | 19       | 0.19          |
| (1,1200) | 1:54:A:LYS:HA   | 1:54:A:LYS:HE3  | 19       | 0.19          |
| (1,1198) | 1:54:A:LYS:HA   | 1:54:A:LYS:HE2  | 19       | 0.19          |
| (1,1198) | 1:54:A:LYS:HA   | 1:54:A:LYS:HE3  | 19       | 0.19          |
| (1,1168) | 1:52:A:HIS:HD2  | 1:52:A:HIS:HB2  | 3        | 0.19          |
| (1,1168) | 1:52:A:HIS:HD2  | 1:52:A:HIS:HB3  | 3        | 0.19          |
| (1,1105) | 1:49:A:LEU:HB2  | 1:52:A:HIS:HD2  | 8        | 0.19          |
| (1,1105) | 1:49:A:LEU:HB3  | 1:52:A:HIS:HD2  | 8        | 0.19          |
| (1,1105) | 1:49:A:LEU:HB2  | 1:52:A:HIS:HD2  | 9        | 0.19          |
| (1,1105) | 1:49:A:LEU:HB3  | 1:52:A:HIS:HD2  | 9        | 0.19          |
| (1,1105) | 1:49:A:LEU:HB2  | 1:52:A:HIS:HD2  | 10       | 0.19          |
| (1,1105) | 1:49:A:LEU:HB3  | 1:52:A:HIS:HD2  | 10       | 0.19          |
| (1,1105) | 1:49:A:LEU:HB2  | 1:52:A:HIS:HD2  | 15       | 0.19          |
| (1,1105) | 1:49:A:LEU:HB3  | 1:52:A:HIS:HD2  | 15       | 0.19          |
| (1,1105) | 1:49:A:LEU:HB2  | 1:52:A:HIS:HD2  | 19       | 0.19          |
| (1,1105) | 1:49:A:LEU:HB3  | 1:52:A:HIS:HD2  | 19       | 0.19          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG21 | 11       | 0.19          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG22 | 11       | 0.19          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG23 | 11       | 0.19          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG21 | 11       | 0.19          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,876) | 1:39:A:ILE:HD12 | 1:40:A:THR:HG22 | 11       | 0.19          |
| (1,876) | 1:39:A:ILE:HD12 | 1:40:A:THR:HG23 | 11       | 0.19          |
| (1,876) | 1:39:A:ILE:HD13 | 1:40:A:THR:HG21 | 11       | 0.19          |
| (1,876) | 1:39:A:ILE:HD13 | 1:40:A:THR:HG22 | 11       | 0.19          |
| (1,876) | 1:39:A:ILE:HD13 | 1:40:A:THR:HG23 | 11       | 0.19          |
| (1,876) | 1:39:A:ILE:HD11 | 1:40:A:THR:HG21 | 13       | 0.19          |
| (1,876) | 1:39:A:ILE:HD11 | 1:40:A:THR:HG22 | 13       | 0.19          |
| (1,876) | 1:39:A:ILE:HD11 | 1:40:A:THR:HG23 | 13       | 0.19          |
| (1,876) | 1:39:A:ILE:HD12 | 1:40:A:THR:HG21 | 13       | 0.19          |
| (1,876) | 1:39:A:ILE:HD12 | 1:40:A:THR:HG22 | 13       | 0.19          |
| (1,876) | 1:39:A:ILE:HD12 | 1:40:A:THR:HG23 | 13       | 0.19          |
| (1,876) | 1:39:A:ILE:HD13 | 1:40:A:THR:HG21 | 13       | 0.19          |
| (1,876) | 1:39:A:ILE:HD13 | 1:40:A:THR:HG22 | 13       | 0.19          |
| (1,876) | 1:39:A:ILE:HD13 | 1:40:A:THR:HG23 | 13       | 0.19          |
| (1,855) | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD11 | 8        | 0.19          |
| (1,855) | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD12 | 8        | 0.19          |
| (1,855) | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD13 | 8        | 0.19          |
| (1,855) | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD11 | 8        | 0.19          |
| (1,855) | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD12 | 8        | 0.19          |
| (1,855) | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD13 | 8        | 0.19          |
| (1,846) | 1:37:A:GLU:HA   | 1:38:A:GLU:H    | 4        | 0.19          |
| (1,846) | 1:37:A:GLU:HA   | 1:38:A:GLU:H    | 12       | 0.19          |
| (1,846) | 1:37:A:GLU:HA   | 1:38:A:GLU:H    | 16       | 0.19          |
| (1,846) | 1:37:A:GLU:HA   | 1:38:A:GLU:H    | 20       | 0.19          |
| (1,815) | 1:35:A:LYS:HD2  | 1:38:A:GLU:HG2  | 8        | 0.19          |
| (1,815) | 1:35:A:LYS:HD2  | 1:38:A:GLU:HG3  | 8        | 0.19          |
| (1,815) | 1:35:A:LYS:HD3  | 1:38:A:GLU:HG2  | 8        | 0.19          |
| (1,815) | 1:35:A:LYS:HD3  | 1:38:A:GLU:HG3  | 8        | 0.19          |
| (1,695) | 1:28:A:LYS:HE2  | 1:29:A:GLU:H    | 14       | 0.19          |
| (1,695) | 1:28:A:LYS:HE3  | 1:29:A:GLU:H    | 14       | 0.19          |
| (1,669) | 1:27:A:CYS:HB2  | 1:30:A:ASP:H    | 3        | 0.19          |
| (1,669) | 1:27:A:CYS:HB3  | 1:30:A:ASP:H    | 3        | 0.19          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG21 | 14       | 0.19          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG22 | 14       | 0.19          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG23 | 14       | 0.19          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG21 | 15       | 0.19          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG22 | 15       | 0.19          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG23 | 15       | 0.19          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG21 | 20       | 0.19          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG22 | 20       | 0.19          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG23 | 20       | 0.19          |
| (1,566) | 1:22:A:GLN:HG2  | 1:25:A:SER:HB2  | 13       | 0.19          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,566) | 1:22:A:GLN:HG2  | 1:25:A:SER:HB3  | 13       | 0.19          |
| (1,566) | 1:22:A:GLN:HG3  | 1:25:A:SER:HB2  | 13       | 0.19          |
| (1,566) | 1:22:A:GLN:HG3  | 1:25:A:SER:HB3  | 13       | 0.19          |
| (1,566) | 1:22:A:GLN:HG2  | 1:25:A:SER:HB2  | 17       | 0.19          |
| (1,566) | 1:22:A:GLN:HG2  | 1:25:A:SER:HB3  | 17       | 0.19          |
| (1,566) | 1:22:A:GLN:HG3  | 1:25:A:SER:HB2  | 17       | 0.19          |
| (1,566) | 1:22:A:GLN:HG3  | 1:25:A:SER:HB3  | 17       | 0.19          |
| (1,566) | 1:22:A:GLN:HG2  | 1:25:A:SER:HB2  | 19       | 0.19          |
| (1,566) | 1:22:A:GLN:HG2  | 1:25:A:SER:HB3  | 19       | 0.19          |
| (1,566) | 1:22:A:GLN:HG3  | 1:25:A:SER:HB2  | 19       | 0.19          |
| (1,566) | 1:22:A:GLN:HG3  | 1:25:A:SER:HB3  | 19       | 0.19          |
| (1,534) | 1:20:A:LEU:HD11 | 1:67:A:PHE:HE1  | 19       | 0.19          |
| (1,534) | 1:20:A:LEU:HD11 | 1:67:A:PHE:HE2  | 19       | 0.19          |
| (1,534) | 1:20:A:LEU:HD12 | 1:67:A:PHE:HE1  | 19       | 0.19          |
| (1,534) | 1:20:A:LEU:HD12 | 1:67:A:PHE:HE2  | 19       | 0.19          |
| (1,534) | 1:20:A:LEU:HD13 | 1:67:A:PHE:HE1  | 19       | 0.19          |
| (1,534) | 1:20:A:LEU:HD13 | 1:67:A:PHE:HE2  | 19       | 0.19          |
| (1,534) | 1:20:A:LEU:HD21 | 1:67:A:PHE:HE1  | 19       | 0.19          |
| (1,534) | 1:20:A:LEU:HD21 | 1:67:A:PHE:HE2  | 19       | 0.19          |
| (1,534) | 1:20:A:LEU:HD22 | 1:67:A:PHE:HE1  | 19       | 0.19          |
| (1,534) | 1:20:A:LEU:HD22 | 1:67:A:PHE:HE2  | 19       | 0.19          |
| (1,534) | 1:20:A:LEU:HD23 | 1:67:A:PHE:HE1  | 19       | 0.19          |
| (1,534) | 1:20:A:LEU:HD23 | 1:67:A:PHE:HE2  | 19       | 0.19          |
| (1,483) | 1:19:A:ASP:HA   | 1:22:A:GLN:HE21 | 11       | 0.19          |
| (1,483) | 1:19:A:ASP:HA   | 1:22:A:GLN:HE22 | 11       | 0.19          |
| (1,483) | 1:19:A:ASP:HA   | 1:22:A:GLN:HE21 | 17       | 0.19          |
| (1,483) | 1:19:A:ASP:HA   | 1:22:A:GLN:HE22 | 17       | 0.19          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB2  | 10       | 0.19          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB3  | 10       | 0.19          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB2  | 10       | 0.19          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB3  | 10       | 0.19          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB2  | 10       | 0.19          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB3  | 10       | 0.19          |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE1  | 2        | 0.19          |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE2  | 2        | 0.19          |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE1  | 19       | 0.19          |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE2  | 19       | 0.19          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD11 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD12 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD13 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD21 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD22 | 5        | 0.19          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD23 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD11 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD12 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD13 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD21 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD22 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD23 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD11 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD12 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD13 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD21 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD22 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD23 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD11 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD12 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD13 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD21 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD22 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD23 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD11 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD12 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD13 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD21 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD22 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD23 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD11 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD12 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD13 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD21 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD22 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD23 | 5        | 0.19          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD11 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD12 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD13 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD21 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD22 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD23 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD11 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD12 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD13 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD21 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD22 | 9        | 0.19          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD23 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD11 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD12 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD13 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD21 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD22 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD23 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD11 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD12 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD13 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD21 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD22 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD23 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD11 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD12 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD13 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD21 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD22 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD23 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD11 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD12 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD13 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD21 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD22 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD23 | 9        | 0.19          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD11 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD12 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD13 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD21 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD22 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD23 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD11 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD12 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD13 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD21 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD22 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD23 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD11 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD12 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD13 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD21 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD22 | 20       | 0.19          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD23 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD11 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD12 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD13 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD21 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD22 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD23 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD11 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD12 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD13 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD21 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD22 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD23 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD11 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD12 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD13 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD21 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD22 | 20       | 0.19          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD23 | 20       | 0.19          |
| (1,127) | 1:6:A:THR:HB    | 1:9:A:GLN:HG2   | 16       | 0.19          |
| (1,127) | 1:6:A:THR:HB    | 1:9:A:GLN:HG3   | 16       | 0.19          |
| (1,112) | 1:6:A:THR:HG21  | 1:6:A:THR:H     | 2        | 0.19          |
| (1,112) | 1:6:A:THR:HG22  | 1:6:A:THR:H     | 2        | 0.19          |
| (1,112) | 1:6:A:THR:HG23  | 1:6:A:THR:H     | 2        | 0.19          |
| (1,112) | 1:6:A:THR:HG21  | 1:6:A:THR:H     | 4        | 0.19          |
| (1,112) | 1:6:A:THR:HG22  | 1:6:A:THR:H     | 4        | 0.19          |
| (1,112) | 1:6:A:THR:HG23  | 1:6:A:THR:H     | 4        | 0.19          |
| (1,112) | 1:6:A:THR:HG21  | 1:6:A:THR:H     | 7        | 0.19          |
| (1,112) | 1:6:A:THR:HG22  | 1:6:A:THR:H     | 7        | 0.19          |
| (1,112) | 1:6:A:THR:HG23  | 1:6:A:THR:H     | 7        | 0.19          |
| (1,112) | 1:6:A:THR:HG21  | 1:6:A:THR:H     | 8        | 0.19          |
| (1,112) | 1:6:A:THR:HG22  | 1:6:A:THR:H     | 8        | 0.19          |
| (1,112) | 1:6:A:THR:HG23  | 1:6:A:THR:H     | 8        | 0.19          |
| (1,112) | 1:6:A:THR:HG21  | 1:6:A:THR:H     | 10       | 0.19          |
| (1,112) | 1:6:A:THR:HG22  | 1:6:A:THR:H     | 10       | 0.19          |
| (1,112) | 1:6:A:THR:HG23  | 1:6:A:THR:H     | 10       | 0.19          |
| (1,112) | 1:6:A:THR:HG21  | 1:6:A:THR:H     | 12       | 0.19          |
| (1,112) | 1:6:A:THR:HG22  | 1:6:A:THR:H     | 12       | 0.19          |
| (1,112) | 1:6:A:THR:HG23  | 1:6:A:THR:H     | 12       | 0.19          |
| (1,112) | 1:6:A:THR:HG21  | 1:6:A:THR:H     | 17       | 0.19          |
| (1,112) | 1:6:A:THR:HG22  | 1:6:A:THR:H     | 17       | 0.19          |
| (1,112) | 1:6:A:THR:HG23  | 1:6:A:THR:H     | 17       | 0.19          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,112)  | 1:6:A:THR:HG21  | 1:6:A:THR:H    | 18       | 0.19          |
| (1,112)  | 1:6:A:THR:HG22  | 1:6:A:THR:H    | 18       | 0.19          |
| (1,112)  | 1:6:A:THR:HG23  | 1:6:A:THR:H    | 18       | 0.19          |
| (1,93)   | 1:4:A:TYR:HA    | 1:82:A:TYR:HE1 | 9        | 0.19          |
| (1,93)   | 1:4:A:TYR:HA    | 1:82:A:TYR:HE2 | 9        | 0.19          |
| (1,20)   | 1:2:A:ALA:HA    | 1:5:A:GLY:H    | 1        | 0.19          |
| (1,20)   | 1:2:A:ALA:HA    | 1:5:A:GLY:H    | 14       | 0.19          |
| (1,20)   | 1:2:A:ALA:HA    | 1:5:A:GLY:H    | 17       | 0.19          |
| (1,6)    | 1:1:A:MET:HA    | 1:3:A:GLU:H    | 18       | 0.19          |
| (1,1762) | 1:82:A:TYR:HE1  | 1:82:A:TYR:H   | 1        | 0.18          |
| (1,1762) | 1:82:A:TYR:HE2  | 1:82:A:TYR:H   | 1        | 0.18          |
| (1,1762) | 1:82:A:TYR:HE1  | 1:82:A:TYR:H   | 5        | 0.18          |
| (1,1762) | 1:82:A:TYR:HE2  | 1:82:A:TYR:H   | 5        | 0.18          |
| (1,1762) | 1:82:A:TYR:HE1  | 1:82:A:TYR:H   | 17       | 0.18          |
| (1,1762) | 1:82:A:TYR:HE2  | 1:82:A:TYR:H   | 17       | 0.18          |
| (1,1762) | 1:82:A:TYR:HE1  | 1:82:A:TYR:H   | 20       | 0.18          |
| (1,1762) | 1:82:A:TYR:HE2  | 1:82:A:TYR:H   | 20       | 0.18          |
| (1,1669) | 1:76:A:LEU:HD11 | 1:80:A:VAL:HB  | 1        | 0.18          |
| (1,1669) | 1:76:A:LEU:HD12 | 1:80:A:VAL:HB  | 1        | 0.18          |
| (1,1669) | 1:76:A:LEU:HD13 | 1:80:A:VAL:HB  | 1        | 0.18          |
| (1,1669) | 1:76:A:LEU:HD21 | 1:80:A:VAL:HB  | 1        | 0.18          |
| (1,1669) | 1:76:A:LEU:HD22 | 1:80:A:VAL:HB  | 1        | 0.18          |
| (1,1669) | 1:76:A:LEU:HD23 | 1:80:A:VAL:HB  | 1        | 0.18          |
| (1,1669) | 1:76:A:LEU:HD11 | 1:80:A:VAL:HB  | 3        | 0.18          |
| (1,1669) | 1:76:A:LEU:HD12 | 1:80:A:VAL:HB  | 3        | 0.18          |
| (1,1669) | 1:76:A:LEU:HD13 | 1:80:A:VAL:HB  | 3        | 0.18          |
| (1,1669) | 1:76:A:LEU:HD21 | 1:80:A:VAL:HB  | 3        | 0.18          |
| (1,1669) | 1:76:A:LEU:HD22 | 1:80:A:VAL:HB  | 3        | 0.18          |
| (1,1669) | 1:76:A:LEU:HD23 | 1:80:A:VAL:HB  | 3        | 0.18          |
| (1,1669) | 1:76:A:LEU:HD11 | 1:80:A:VAL:HB  | 5        | 0.18          |
| (1,1669) | 1:76:A:LEU:HD12 | 1:80:A:VAL:HB  | 5        | 0.18          |
| (1,1669) | 1:76:A:LEU:HD13 | 1:80:A:VAL:HB  | 5        | 0.18          |
| (1,1669) | 1:76:A:LEU:HD21 | 1:80:A:VAL:HB  | 5        | 0.18          |
| (1,1669) | 1:76:A:LEU:HD22 | 1:80:A:VAL:HB  | 5        | 0.18          |
| (1,1669) | 1:76:A:LEU:HD23 | 1:80:A:VAL:HB  | 5        | 0.18          |
| (1,1669) | 1:76:A:LEU:HD11 | 1:80:A:VAL:HB  | 10       | 0.18          |
| (1,1669) | 1:76:A:LEU:HD12 | 1:80:A:VAL:HB  | 10       | 0.18          |
| (1,1669) | 1:76:A:LEU:HD13 | 1:80:A:VAL:HB  | 10       | 0.18          |
| (1,1669) | 1:76:A:LEU:HD21 | 1:80:A:VAL:HB  | 10       | 0.18          |
| (1,1669) | 1:76:A:LEU:HD22 | 1:80:A:VAL:HB  | 10       | 0.18          |
| (1,1669) | 1:76:A:LEU:HD23 | 1:80:A:VAL:HB  | 10       | 0.18          |
| (1,1669) | 1:76:A:LEU:HD11 | 1:80:A:VAL:HB  | 11       | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1669) | 1:76:A:LEU:HD12 | 1:80:A:VAL:HB   | 11       | 0.18          |
| (1,1669) | 1:76:A:LEU:HD13 | 1:80:A:VAL:HB   | 11       | 0.18          |
| (1,1669) | 1:76:A:LEU:HD21 | 1:80:A:VAL:HB   | 11       | 0.18          |
| (1,1669) | 1:76:A:LEU:HD22 | 1:80:A:VAL:HB   | 11       | 0.18          |
| (1,1669) | 1:76:A:LEU:HD23 | 1:80:A:VAL:HB   | 11       | 0.18          |
| (1,1669) | 1:76:A:LEU:HD11 | 1:80:A:VAL:HB   | 13       | 0.18          |
| (1,1669) | 1:76:A:LEU:HD12 | 1:80:A:VAL:HB   | 13       | 0.18          |
| (1,1669) | 1:76:A:LEU:HD13 | 1:80:A:VAL:HB   | 13       | 0.18          |
| (1,1669) | 1:76:A:LEU:HD21 | 1:80:A:VAL:HB   | 13       | 0.18          |
| (1,1669) | 1:76:A:LEU:HD22 | 1:80:A:VAL:HB   | 13       | 0.18          |
| (1,1669) | 1:76:A:LEU:HD23 | 1:80:A:VAL:HB   | 13       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG11 | 1        | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG12 | 1        | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG13 | 1        | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG21 | 1        | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG22 | 1        | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG23 | 1        | 0.18          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG11 | 1        | 0.18          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG12 | 1        | 0.18          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG13 | 1        | 0.18          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG21 | 1        | 0.18          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG22 | 1        | 0.18          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG23 | 1        | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG11 | 8        | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG12 | 8        | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG13 | 8        | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG21 | 8        | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG22 | 8        | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG23 | 8        | 0.18          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG11 | 8        | 0.18          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG12 | 8        | 0.18          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG13 | 8        | 0.18          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG21 | 8        | 0.18          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG22 | 8        | 0.18          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG23 | 8        | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG11 | 10       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG12 | 10       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG13 | 10       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG21 | 10       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG22 | 10       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG23 | 10       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG11 | 10       | 0.18          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG12 | 10       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG13 | 10       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG21 | 10       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG22 | 10       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG23 | 10       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG11 | 12       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG12 | 12       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG13 | 12       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG21 | 12       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG22 | 12       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG23 | 12       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG11 | 12       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG12 | 12       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG13 | 12       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG21 | 12       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG22 | 12       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG23 | 12       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG11 | 14       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG12 | 14       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG13 | 14       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG21 | 14       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG22 | 14       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB2 | 1:80:A:VAL:HG23 | 14       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG11 | 14       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG12 | 14       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG13 | 14       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG21 | 14       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG22 | 14       | 0.18          |
| (1,1666) | 1:76:A:LEU:HB3 | 1:80:A:VAL:HG23 | 14       | 0.18          |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD11 | 11       | 0.18          |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD12 | 11       | 0.18          |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD13 | 11       | 0.18          |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD11 | 19       | 0.18          |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD12 | 19       | 0.18          |
| (1,1550) | 1:69:A:ILE:HA  | 1:69:A:ILE:HD13 | 19       | 0.18          |
| (1,1541) | 1:68:A:GLU:HG2 | 1:76:A:LEU:HD11 | 19       | 0.18          |
| (1,1541) | 1:68:A:GLU:HG2 | 1:76:A:LEU:HD12 | 19       | 0.18          |
| (1,1541) | 1:68:A:GLU:HG2 | 1:76:A:LEU:HD13 | 19       | 0.18          |
| (1,1541) | 1:68:A:GLU:HG2 | 1:76:A:LEU:HD21 | 19       | 0.18          |
| (1,1541) | 1:68:A:GLU:HG2 | 1:76:A:LEU:HD22 | 19       | 0.18          |
| (1,1541) | 1:68:A:GLU:HG2 | 1:76:A:LEU:HD23 | 19       | 0.18          |
| (1,1541) | 1:68:A:GLU:HG3 | 1:76:A:LEU:HD11 | 19       | 0.18          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1541) | 1:68:A:GLU:HG3 | 1:76:A:LEU:HD12 | 19       | 0.18          |
| (1,1541) | 1:68:A:GLU:HG3 | 1:76:A:LEU:HD13 | 19       | 0.18          |
| (1,1541) | 1:68:A:GLU:HG3 | 1:76:A:LEU:HD21 | 19       | 0.18          |
| (1,1541) | 1:68:A:GLU:HG3 | 1:76:A:LEU:HD22 | 19       | 0.18          |
| (1,1541) | 1:68:A:GLU:HG3 | 1:76:A:LEU:HD23 | 19       | 0.18          |
| (1,1454) | 1:66:A:ILE:HA  | 1:67:A:PHE:H    | 2        | 0.18          |
| (1,1454) | 1:66:A:ILE:HA  | 1:67:A:PHE:H    | 6        | 0.18          |
| (1,1454) | 1:66:A:ILE:HA  | 1:67:A:PHE:H    | 7        | 0.18          |
| (1,1454) | 1:66:A:ILE:HA  | 1:67:A:PHE:H    | 14       | 0.18          |
| (1,1454) | 1:66:A:ILE:HA  | 1:67:A:PHE:H    | 15       | 0.18          |
| (1,1454) | 1:66:A:ILE:HA  | 1:67:A:PHE:H    | 17       | 0.18          |
| (1,1439) | 1:65:A:HIS:HA  | 1:69:A:ILE:H    | 20       | 0.18          |
| (1,1437) | 1:65:A:HIS:HA  | 1:68:A:GLU:H    | 15       | 0.18          |
| (1,1428) | 1:65:A:HIS:HD2 | 1:66:A:ILE:HG12 | 2        | 0.18          |
| (1,1428) | 1:65:A:HIS:HD2 | 1:66:A:ILE:HG13 | 2        | 0.18          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD11 | 6        | 0.18          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD12 | 6        | 0.18          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD13 | 6        | 0.18          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD11 | 9        | 0.18          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD12 | 9        | 0.18          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD13 | 9        | 0.18          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD11 | 10       | 0.18          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD12 | 10       | 0.18          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD13 | 10       | 0.18          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD11 | 12       | 0.18          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD12 | 12       | 0.18          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD13 | 12       | 0.18          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD11 | 19       | 0.18          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD12 | 19       | 0.18          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD13 | 19       | 0.18          |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG12 | 6        | 0.18          |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG13 | 6        | 0.18          |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG12 | 6        | 0.18          |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG13 | 6        | 0.18          |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG12 | 11       | 0.18          |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG13 | 11       | 0.18          |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG12 | 11       | 0.18          |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG13 | 11       | 0.18          |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG12 | 16       | 0.18          |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG13 | 16       | 0.18          |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG12 | 16       | 0.18          |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG13 | 16       | 0.18          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG21 | 1        | 0.18          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG22 | 1        | 0.18          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG23 | 1        | 0.18          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG21 | 11       | 0.18          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG22 | 11       | 0.18          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG23 | 11       | 0.18          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG21 | 17       | 0.18          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG22 | 17       | 0.18          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG23 | 17       | 0.18          |
| (1,1277) | 1:58:A:ASP:H   | 1:60:A:LEU:H    | 9        | 0.18          |
| (1,1274) | 1:58:A:ASP:H   | 1:59:A:ASN:HD21 | 11       | 0.18          |
| (1,1274) | 1:58:A:ASP:H   | 1:59:A:ASN:HD22 | 11       | 0.18          |
| (1,1273) | 1:58:A:ASP:HA  | 1:59:A:ASN:HD21 | 20       | 0.18          |
| (1,1273) | 1:58:A:ASP:HA  | 1:59:A:ASN:HD22 | 20       | 0.18          |
| (1,1267) | 1:57:A:LYS:HD2 | 1:59:A:ASN:H    | 12       | 0.18          |
| (1,1267) | 1:57:A:LYS:HD3 | 1:59:A:ASN:H    | 12       | 0.18          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD2  | 15       | 0.18          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD3  | 15       | 0.18          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD2  | 17       | 0.18          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD3  | 17       | 0.18          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG2  | 6        | 0.18          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG3  | 6        | 0.18          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG2  | 20       | 0.18          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG3  | 20       | 0.18          |
| (1,1211) | 1:54:A:LYS:HB2 | 1:62:A:TYR:H    | 17       | 0.18          |
| (1,1211) | 1:54:A:LYS:HB3 | 1:62:A:TYR:H    | 17       | 0.18          |
| (1,1211) | 1:54:A:LYS:HB2 | 1:62:A:TYR:H    | 18       | 0.18          |
| (1,1211) | 1:54:A:LYS:HB3 | 1:62:A:TYR:H    | 18       | 0.18          |
| (1,1207) | 1:54:A:LYS:HG2 | 1:62:A:TYR:HE1  | 5        | 0.18          |
| (1,1207) | 1:54:A:LYS:HG2 | 1:62:A:TYR:HE2  | 5        | 0.18          |
| (1,1207) | 1:54:A:LYS:HG3 | 1:62:A:TYR:HE1  | 5        | 0.18          |
| (1,1207) | 1:54:A:LYS:HG3 | 1:62:A:TYR:HE2  | 5        | 0.18          |
| (1,1168) | 1:52:A:HIS:HD2 | 1:52:A:HIS:HB2  | 8        | 0.18          |
| (1,1168) | 1:52:A:HIS:HD2 | 1:52:A:HIS:HB3  | 8        | 0.18          |
| (1,1168) | 1:52:A:HIS:HD2 | 1:52:A:HIS:HB2  | 14       | 0.18          |
| (1,1168) | 1:52:A:HIS:HD2 | 1:52:A:HIS:HB3  | 14       | 0.18          |
| (1,1168) | 1:52:A:HIS:HD2 | 1:52:A:HIS:HB2  | 16       | 0.18          |
| (1,1168) | 1:52:A:HIS:HD2 | 1:52:A:HIS:HB3  | 16       | 0.18          |
| (1,1168) | 1:52:A:HIS:HD2 | 1:52:A:HIS:HB2  | 18       | 0.18          |
| (1,1168) | 1:52:A:HIS:HD2 | 1:52:A:HIS:HB3  | 18       | 0.18          |
| (1,1168) | 1:52:A:HIS:HD2 | 1:52:A:HIS:HB2  | 19       | 0.18          |
| (1,1168) | 1:52:A:HIS:HD2 | 1:52:A:HIS:HB3  | 19       | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1168) | 1:52:A:HIS:HD2  | 1:52:A:HIS:HB2  | 20       | 0.18          |
| (1,1168) | 1:52:A:HIS:HD2  | 1:52:A:HIS:HB3  | 20       | 0.18          |
| (1,1105) | 1:49:A:LEU:HB2  | 1:52:A:HIS:HD2  | 17       | 0.18          |
| (1,1105) | 1:49:A:LEU:HB3  | 1:52:A:HIS:HD2  | 17       | 0.18          |
| (1,1105) | 1:49:A:LEU:HB2  | 1:52:A:HIS:HD2  | 18       | 0.18          |
| (1,1105) | 1:49:A:LEU:HB3  | 1:52:A:HIS:HD2  | 18       | 0.18          |
| (1,997)  | 1:45:A:TRP:HA   | 1:50:A:GLU:H    | 7        | 0.18          |
| (1,894)  | 1:39:A:ILE:HD11 | 1:45:A:TRP:HH2  | 20       | 0.18          |
| (1,894)  | 1:39:A:ILE:HD12 | 1:45:A:TRP:HH2  | 20       | 0.18          |
| (1,894)  | 1:39:A:ILE:HD13 | 1:45:A:TRP:HH2  | 20       | 0.18          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG21 | 1        | 0.18          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG22 | 1        | 0.18          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG23 | 1        | 0.18          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG21 | 1        | 0.18          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG22 | 1        | 0.18          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG23 | 1        | 0.18          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG21 | 1        | 0.18          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG22 | 1        | 0.18          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG23 | 1        | 0.18          |
| (1,855)  | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD11 | 6        | 0.18          |
| (1,855)  | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD12 | 6        | 0.18          |
| (1,855)  | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD13 | 6        | 0.18          |
| (1,855)  | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD11 | 6        | 0.18          |
| (1,855)  | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD12 | 6        | 0.18          |
| (1,855)  | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD13 | 6        | 0.18          |
| (1,846)  | 1:37:A:GLU:HA   | 1:38:A:GLU:H    | 10       | 0.18          |
| (1,844)  | 1:37:A:GLU:H    | 1:38:A:GLU:H    | 1        | 0.18          |
| (1,844)  | 1:37:A:GLU:H    | 1:38:A:GLU:H    | 4        | 0.18          |
| (1,844)  | 1:37:A:GLU:H    | 1:38:A:GLU:H    | 16       | 0.18          |
| (1,844)  | 1:37:A:GLU:H    | 1:38:A:GLU:H    | 20       | 0.18          |
| (1,772)  | 1:31:A:ILE:HG21 | 1:49:A:LEU:HA   | 5        | 0.18          |
| (1,772)  | 1:31:A:ILE:HG22 | 1:49:A:LEU:HA   | 5        | 0.18          |
| (1,772)  | 1:31:A:ILE:HG23 | 1:49:A:LEU:HA   | 5        | 0.18          |
| (1,772)  | 1:31:A:ILE:HG21 | 1:49:A:LEU:HA   | 13       | 0.18          |
| (1,772)  | 1:31:A:ILE:HG22 | 1:49:A:LEU:HA   | 13       | 0.18          |
| (1,772)  | 1:31:A:ILE:HG23 | 1:49:A:LEU:HA   | 13       | 0.18          |
| (1,772)  | 1:31:A:ILE:HG21 | 1:49:A:LEU:HA   | 17       | 0.18          |
| (1,772)  | 1:31:A:ILE:HG22 | 1:49:A:LEU:HA   | 17       | 0.18          |
| (1,772)  | 1:31:A:ILE:HG23 | 1:49:A:LEU:HA   | 17       | 0.18          |
| (1,743)  | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD2  | 1        | 0.18          |
| (1,743)  | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD3  | 1        | 0.18          |
| (1,743)  | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD2  | 1        | 0.18          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,743) | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD3  | 1        | 0.18          |
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD2  | 1        | 0.18          |
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD3  | 1        | 0.18          |
| (1,743) | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD2  | 8        | 0.18          |
| (1,743) | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD3  | 8        | 0.18          |
| (1,743) | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD2  | 8        | 0.18          |
| (1,743) | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD3  | 8        | 0.18          |
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD2  | 8        | 0.18          |
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD3  | 8        | 0.18          |
| (1,743) | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD2  | 9        | 0.18          |
| (1,743) | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD3  | 9        | 0.18          |
| (1,743) | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD2  | 9        | 0.18          |
| (1,743) | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD3  | 9        | 0.18          |
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD2  | 9        | 0.18          |
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD3  | 9        | 0.18          |
| (1,669) | 1:27:A:CYS:HB2  | 1:30:A:ASP:H    | 19       | 0.18          |
| (1,669) | 1:27:A:CYS:HB3  | 1:30:A:ASP:H    | 19       | 0.18          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG21 | 8        | 0.18          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG22 | 8        | 0.18          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG23 | 8        | 0.18          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG21 | 19       | 0.18          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG22 | 19       | 0.18          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG23 | 19       | 0.18          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB2  | 6        | 0.18          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB3  | 6        | 0.18          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB2  | 6        | 0.18          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB3  | 6        | 0.18          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB2  | 6        | 0.18          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB3  | 6        | 0.18          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB2  | 17       | 0.18          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB3  | 17       | 0.18          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB2  | 17       | 0.18          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB3  | 17       | 0.18          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB2  | 17       | 0.18          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB3  | 17       | 0.18          |
| (1,425) | 1:16:A:THR:HG21 | 1:18:A:GLU:H    | 7        | 0.18          |
| (1,425) | 1:16:A:THR:HG22 | 1:18:A:GLU:H    | 7        | 0.18          |
| (1,425) | 1:16:A:THR:HG23 | 1:18:A:GLU:H    | 7        | 0.18          |
| (1,425) | 1:16:A:THR:HG21 | 1:18:A:GLU:H    | 8        | 0.18          |
| (1,425) | 1:16:A:THR:HG22 | 1:18:A:GLU:H    | 8        | 0.18          |
| (1,425) | 1:16:A:THR:HG23 | 1:18:A:GLU:H    | 8        | 0.18          |
| (1,425) | 1:16:A:THR:HG21 | 1:18:A:GLU:H    | 10       | 0.18          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,425) | 1:16:A:THR:HG22 | 1:18:A:GLU:H    | 10       | 0.18          |
| (1,425) | 1:16:A:THR:HG23 | 1:18:A:GLU:H    | 10       | 0.18          |
| (1,425) | 1:16:A:THR:HG21 | 1:18:A:GLU:H    | 15       | 0.18          |
| (1,425) | 1:16:A:THR:HG22 | 1:18:A:GLU:H    | 15       | 0.18          |
| (1,425) | 1:16:A:THR:HG23 | 1:18:A:GLU:H    | 15       | 0.18          |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE1  | 10       | 0.18          |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE2  | 10       | 0.18          |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE1  | 16       | 0.18          |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE2  | 16       | 0.18          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD1  | 1        | 0.18          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD2  | 1        | 0.18          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD1  | 1        | 0.18          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD2  | 1        | 0.18          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD1  | 1        | 0.18          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD2  | 1        | 0.18          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD1  | 3        | 0.18          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD2  | 3        | 0.18          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD1  | 3        | 0.18          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD2  | 3        | 0.18          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD1  | 3        | 0.18          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD2  | 3        | 0.18          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD1  | 6        | 0.18          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD2  | 6        | 0.18          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD1  | 6        | 0.18          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD2  | 6        | 0.18          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD1  | 6        | 0.18          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD2  | 6        | 0.18          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD1  | 15       | 0.18          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD2  | 15       | 0.18          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD1  | 15       | 0.18          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD2  | 15       | 0.18          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD1  | 15       | 0.18          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD2  | 15       | 0.18          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG21 | 1        | 0.18          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG22 | 1        | 0.18          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG23 | 1        | 0.18          |
| (1,245) | 1:9:A:GLN:HE22  | 1:12:A:THR:HG21 | 1        | 0.18          |
| (1,245) | 1:9:A:GLN:HE22  | 1:12:A:THR:HG22 | 1        | 0.18          |
| (1,245) | 1:9:A:GLN:HE22  | 1:12:A:THR:HG23 | 1        | 0.18          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG21 | 7        | 0.18          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG22 | 7        | 0.18          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG23 | 7        | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,245)  | 1:9:A:GLN:HE22  | 1:12:A:THR:HG21 | 7        | 0.18          |
| (1,245)  | 1:9:A:GLN:HE22  | 1:12:A:THR:HG22 | 7        | 0.18          |
| (1,245)  | 1:9:A:GLN:HE22  | 1:12:A:THR:HG23 | 7        | 0.18          |
| (1,245)  | 1:9:A:GLN:HE21  | 1:12:A:THR:HG21 | 12       | 0.18          |
| (1,245)  | 1:9:A:GLN:HE21  | 1:12:A:THR:HG22 | 12       | 0.18          |
| (1,245)  | 1:9:A:GLN:HE21  | 1:12:A:THR:HG23 | 12       | 0.18          |
| (1,245)  | 1:9:A:GLN:HE22  | 1:12:A:THR:HG21 | 12       | 0.18          |
| (1,245)  | 1:9:A:GLN:HE22  | 1:12:A:THR:HG22 | 12       | 0.18          |
| (1,245)  | 1:9:A:GLN:HE22  | 1:12:A:THR:HG23 | 12       | 0.18          |
| (1,245)  | 1:9:A:GLN:HE21  | 1:12:A:THR:HG21 | 20       | 0.18          |
| (1,245)  | 1:9:A:GLN:HE21  | 1:12:A:THR:HG22 | 20       | 0.18          |
| (1,245)  | 1:9:A:GLN:HE21  | 1:12:A:THR:HG23 | 20       | 0.18          |
| (1,245)  | 1:9:A:GLN:HE22  | 1:12:A:THR:HG21 | 20       | 0.18          |
| (1,245)  | 1:9:A:GLN:HE22  | 1:12:A:THR:HG22 | 20       | 0.18          |
| (1,245)  | 1:9:A:GLN:HE22  | 1:12:A:THR:HG23 | 20       | 0.18          |
| (1,112)  | 1:6:A:THR:HG21  | 1:6:A:THR:H     | 6        | 0.18          |
| (1,112)  | 1:6:A:THR:HG22  | 1:6:A:THR:H     | 6        | 0.18          |
| (1,112)  | 1:6:A:THR:HG23  | 1:6:A:THR:H     | 6        | 0.18          |
| (1,112)  | 1:6:A:THR:HG21  | 1:6:A:THR:H     | 9        | 0.18          |
| (1,112)  | 1:6:A:THR:HG22  | 1:6:A:THR:H     | 9        | 0.18          |
| (1,112)  | 1:6:A:THR:HG23  | 1:6:A:THR:H     | 9        | 0.18          |
| (1,112)  | 1:6:A:THR:HG21  | 1:6:A:THR:H     | 11       | 0.18          |
| (1,112)  | 1:6:A:THR:HG22  | 1:6:A:THR:H     | 11       | 0.18          |
| (1,112)  | 1:6:A:THR:HG23  | 1:6:A:THR:H     | 11       | 0.18          |
| (1,112)  | 1:6:A:THR:HG21  | 1:6:A:THR:H     | 16       | 0.18          |
| (1,112)  | 1:6:A:THR:HG22  | 1:6:A:THR:H     | 16       | 0.18          |
| (1,112)  | 1:6:A:THR:HG23  | 1:6:A:THR:H     | 16       | 0.18          |
| (1,112)  | 1:6:A:THR:HG21  | 1:6:A:THR:H     | 20       | 0.18          |
| (1,112)  | 1:6:A:THR:HG22  | 1:6:A:THR:H     | 20       | 0.18          |
| (1,112)  | 1:6:A:THR:HG23  | 1:6:A:THR:H     | 20       | 0.18          |
| (1,93)   | 1:4:A:TYR:HA    | 1:82:A:TYR:HE1  | 12       | 0.18          |
| (1,93)   | 1:4:A:TYR:HA    | 1:82:A:TYR:HE2  | 12       | 0.18          |
| (1,20)   | 1:2:A:ALA:HA    | 1:5:A:GLY:H     | 5        | 0.18          |
| (1,10)   | 1:1:A:MET:HA    | 1:57:A:LYS:HD2  | 11       | 0.18          |
| (1,10)   | 1:1:A:MET:HA    | 1:57:A:LYS:HD3  | 11       | 0.18          |
| (1,6)    | 1:1:A:MET:HA    | 1:3:A:GLU:H     | 12       | 0.18          |
| (1,1888) | 1:89:A:ILE:HG21 | 1:89:A:ILE:H    | 3        | 0.17          |
| (1,1888) | 1:89:A:ILE:HG22 | 1:89:A:ILE:H    | 3        | 0.17          |
| (1,1888) | 1:89:A:ILE:HG23 | 1:89:A:ILE:H    | 3        | 0.17          |
| (1,1888) | 1:89:A:ILE:HG21 | 1:89:A:ILE:H    | 5        | 0.17          |
| (1,1888) | 1:89:A:ILE:HG22 | 1:89:A:ILE:H    | 5        | 0.17          |
| (1,1888) | 1:89:A:ILE:HG23 | 1:89:A:ILE:H    | 5        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1884) | 1:88:A:LYS:HD2  | 1:89:A:ILE:H    | 15       | 0.17          |
| (1,1884) | 1:88:A:LYS:HD3  | 1:89:A:ILE:H    | 15       | 0.17          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD2  | 5        | 0.17          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD3  | 5        | 0.17          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD2  | 5        | 0.17          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD3  | 5        | 0.17          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD2  | 5        | 0.17          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD3  | 5        | 0.17          |
| (1,1796) | 1:83:A:ARG:HD2  | 1:84:A:THR:HG21 | 13       | 0.17          |
| (1,1796) | 1:83:A:ARG:HD2  | 1:84:A:THR:HG22 | 13       | 0.17          |
| (1,1796) | 1:83:A:ARG:HD2  | 1:84:A:THR:HG23 | 13       | 0.17          |
| (1,1796) | 1:83:A:ARG:HD3  | 1:84:A:THR:HG21 | 13       | 0.17          |
| (1,1796) | 1:83:A:ARG:HD3  | 1:84:A:THR:HG22 | 13       | 0.17          |
| (1,1796) | 1:83:A:ARG:HD3  | 1:84:A:THR:HG23 | 13       | 0.17          |
| (1,1794) | 1:83:A:ARG:HG2  | 1:84:A:THR:H    | 12       | 0.17          |
| (1,1794) | 1:83:A:ARG:HG3  | 1:84:A:THR:H    | 12       | 0.17          |
| (1,1794) | 1:83:A:ARG:HG2  | 1:84:A:THR:H    | 13       | 0.17          |
| (1,1794) | 1:83:A:ARG:HG3  | 1:84:A:THR:H    | 13       | 0.17          |
| (1,1762) | 1:82:A:TYR:HE1  | 1:82:A:TYR:H    | 3        | 0.17          |
| (1,1762) | 1:82:A:TYR:HE2  | 1:82:A:TYR:H    | 3        | 0.17          |
| (1,1762) | 1:82:A:TYR:HE1  | 1:82:A:TYR:H    | 4        | 0.17          |
| (1,1762) | 1:82:A:TYR:HE2  | 1:82:A:TYR:H    | 4        | 0.17          |
| (1,1762) | 1:82:A:TYR:HE1  | 1:82:A:TYR:H    | 7        | 0.17          |
| (1,1762) | 1:82:A:TYR:HE2  | 1:82:A:TYR:H    | 7        | 0.17          |
| (1,1762) | 1:82:A:TYR:HE1  | 1:82:A:TYR:H    | 8        | 0.17          |
| (1,1762) | 1:82:A:TYR:HE2  | 1:82:A:TYR:H    | 8        | 0.17          |
| (1,1762) | 1:82:A:TYR:HE1  | 1:82:A:TYR:H    | 9        | 0.17          |
| (1,1762) | 1:82:A:TYR:HE2  | 1:82:A:TYR:H    | 9        | 0.17          |
| (1,1762) | 1:82:A:TYR:HE1  | 1:82:A:TYR:H    | 12       | 0.17          |
| (1,1762) | 1:82:A:TYR:HE2  | 1:82:A:TYR:H    | 12       | 0.17          |
| (1,1762) | 1:82:A:TYR:HE1  | 1:82:A:TYR:H    | 19       | 0.17          |
| (1,1762) | 1:82:A:TYR:HE2  | 1:82:A:TYR:H    | 19       | 0.17          |
| (1,1745) | 1:80:A:VAL:HA   | 1:83:A:ARG:HD2  | 6        | 0.17          |
| (1,1745) | 1:80:A:VAL:HA   | 1:83:A:ARG:HD3  | 6        | 0.17          |
| (1,1669) | 1:76:A:LEU:HD11 | 1:80:A:VAL:HB   | 6        | 0.17          |
| (1,1669) | 1:76:A:LEU:HD12 | 1:80:A:VAL:HB   | 6        | 0.17          |
| (1,1669) | 1:76:A:LEU:HD13 | 1:80:A:VAL:HB   | 6        | 0.17          |
| (1,1669) | 1:76:A:LEU:HD21 | 1:80:A:VAL:HB   | 6        | 0.17          |
| (1,1669) | 1:76:A:LEU:HD22 | 1:80:A:VAL:HB   | 6        | 0.17          |
| (1,1669) | 1:76:A:LEU:HD23 | 1:80:A:VAL:HB   | 6        | 0.17          |
| (1,1669) | 1:76:A:LEU:HD11 | 1:80:A:VAL:HB   | 7        | 0.17          |
| (1,1669) | 1:76:A:LEU:HD12 | 1:80:A:VAL:HB   | 7        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1669) | 1:76:A:LEU:HD13 | 1:80:A:VAL:HB   | 7        | 0.17          |
| (1,1669) | 1:76:A:LEU:HD21 | 1:80:A:VAL:HB   | 7        | 0.17          |
| (1,1669) | 1:76:A:LEU:HD22 | 1:80:A:VAL:HB   | 7        | 0.17          |
| (1,1669) | 1:76:A:LEU:HD23 | 1:80:A:VAL:HB   | 7        | 0.17          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG11 | 6        | 0.17          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG12 | 6        | 0.17          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG13 | 6        | 0.17          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG21 | 6        | 0.17          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG22 | 6        | 0.17          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG23 | 6        | 0.17          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG11 | 6        | 0.17          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG12 | 6        | 0.17          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG13 | 6        | 0.17          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG21 | 6        | 0.17          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG22 | 6        | 0.17          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG23 | 6        | 0.17          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG11 | 7        | 0.17          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG12 | 7        | 0.17          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG13 | 7        | 0.17          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG21 | 7        | 0.17          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG22 | 7        | 0.17          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG23 | 7        | 0.17          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG11 | 7        | 0.17          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG12 | 7        | 0.17          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG13 | 7        | 0.17          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG21 | 7        | 0.17          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG22 | 7        | 0.17          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG23 | 7        | 0.17          |
| (1,1597) | 1:72:A:ARG:HG2  | 1:74:A:ASP:H    | 2        | 0.17          |
| (1,1597) | 1:72:A:ARG:HG3  | 1:74:A:ASP:H    | 2        | 0.17          |
| (1,1541) | 1:68:A:GLU:HG2  | 1:76:A:LEU:HD11 | 3        | 0.17          |
| (1,1541) | 1:68:A:GLU:HG2  | 1:76:A:LEU:HD12 | 3        | 0.17          |
| (1,1541) | 1:68:A:GLU:HG2  | 1:76:A:LEU:HD13 | 3        | 0.17          |
| (1,1541) | 1:68:A:GLU:HG2  | 1:76:A:LEU:HD21 | 3        | 0.17          |
| (1,1541) | 1:68:A:GLU:HG2  | 1:76:A:LEU:HD22 | 3        | 0.17          |
| (1,1541) | 1:68:A:GLU:HG2  | 1:76:A:LEU:HD23 | 3        | 0.17          |
| (1,1541) | 1:68:A:GLU:HG3  | 1:76:A:LEU:HD11 | 3        | 0.17          |
| (1,1541) | 1:68:A:GLU:HG3  | 1:76:A:LEU:HD12 | 3        | 0.17          |
| (1,1541) | 1:68:A:GLU:HG3  | 1:76:A:LEU:HD13 | 3        | 0.17          |
| (1,1541) | 1:68:A:GLU:HG3  | 1:76:A:LEU:HD21 | 3        | 0.17          |
| (1,1541) | 1:68:A:GLU:HG3  | 1:76:A:LEU:HD22 | 3        | 0.17          |
| (1,1541) | 1:68:A:GLU:HG3  | 1:76:A:LEU:HD23 | 3        | 0.17          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1541) | 1:68:A:GLU:HG2 | 1:76:A:LEU:HD11 | 4        | 0.17          |
| (1,1541) | 1:68:A:GLU:HG2 | 1:76:A:LEU:HD12 | 4        | 0.17          |
| (1,1541) | 1:68:A:GLU:HG2 | 1:76:A:LEU:HD13 | 4        | 0.17          |
| (1,1541) | 1:68:A:GLU:HG2 | 1:76:A:LEU:HD21 | 4        | 0.17          |
| (1,1541) | 1:68:A:GLU:HG2 | 1:76:A:LEU:HD22 | 4        | 0.17          |
| (1,1541) | 1:68:A:GLU:HG2 | 1:76:A:LEU:HD23 | 4        | 0.17          |
| (1,1541) | 1:68:A:GLU:HG3 | 1:76:A:LEU:HD11 | 4        | 0.17          |
| (1,1541) | 1:68:A:GLU:HG3 | 1:76:A:LEU:HD12 | 4        | 0.17          |
| (1,1541) | 1:68:A:GLU:HG3 | 1:76:A:LEU:HD13 | 4        | 0.17          |
| (1,1541) | 1:68:A:GLU:HG3 | 1:76:A:LEU:HD21 | 4        | 0.17          |
| (1,1541) | 1:68:A:GLU:HG3 | 1:76:A:LEU:HD22 | 4        | 0.17          |
| (1,1541) | 1:68:A:GLU:HG3 | 1:76:A:LEU:HD23 | 4        | 0.17          |
| (1,1525) | 1:68:A:GLU:HA  | 1:68:A:GLU:HG2  | 12       | 0.17          |
| (1,1525) | 1:68:A:GLU:HA  | 1:68:A:GLU:HG3  | 12       | 0.17          |
| (1,1516) | 1:67:A:PHE:H   | 1:76:A:LEU:HG   | 2        | 0.17          |
| (1,1516) | 1:67:A:PHE:H   | 1:76:A:LEU:HG   | 15       | 0.17          |
| (1,1454) | 1:66:A:ILE:HA  | 1:67:A:PHE:H    | 1        | 0.17          |
| (1,1454) | 1:66:A:ILE:HA  | 1:67:A:PHE:H    | 3        | 0.17          |
| (1,1454) | 1:66:A:ILE:HA  | 1:67:A:PHE:H    | 5        | 0.17          |
| (1,1454) | 1:66:A:ILE:HA  | 1:67:A:PHE:H    | 8        | 0.17          |
| (1,1454) | 1:66:A:ILE:HA  | 1:67:A:PHE:H    | 9        | 0.17          |
| (1,1454) | 1:66:A:ILE:HA  | 1:67:A:PHE:H    | 12       | 0.17          |
| (1,1454) | 1:66:A:ILE:HA  | 1:67:A:PHE:H    | 13       | 0.17          |
| (1,1439) | 1:65:A:HIS:HA  | 1:69:A:ILE:H    | 2        | 0.17          |
| (1,1428) | 1:65:A:HIS:HD2 | 1:66:A:ILE:HG12 | 5        | 0.17          |
| (1,1428) | 1:65:A:HIS:HD2 | 1:66:A:ILE:HG13 | 5        | 0.17          |
| (1,1428) | 1:65:A:HIS:HD2 | 1:66:A:ILE:HG12 | 18       | 0.17          |
| (1,1428) | 1:65:A:HIS:HD2 | 1:66:A:ILE:HG13 | 18       | 0.17          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD11 | 5        | 0.17          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD12 | 5        | 0.17          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD13 | 5        | 0.17          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD11 | 11       | 0.17          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD12 | 11       | 0.17          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD13 | 11       | 0.17          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD11 | 17       | 0.17          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD12 | 17       | 0.17          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD13 | 17       | 0.17          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD11 | 18       | 0.17          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD12 | 18       | 0.17          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD13 | 18       | 0.17          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD11 | 20       | 0.17          |
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD12 | 20       | 0.17          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1357) | 1:63:A:ILE:HA  | 1:63:A:ILE:HD13 | 20       | 0.17          |
| (1,1355) | 1:63:A:ILE:HB  | 1:63:A:ILE:H    | 20       | 0.17          |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG12 | 17       | 0.17          |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG13 | 17       | 0.17          |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG12 | 17       | 0.17          |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG13 | 17       | 0.17          |
| (1,1349) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HD11 | 5        | 0.17          |
| (1,1349) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HD12 | 5        | 0.17          |
| (1,1349) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HD13 | 5        | 0.17          |
| (1,1349) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HD11 | 5        | 0.17          |
| (1,1349) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HD12 | 5        | 0.17          |
| (1,1349) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HD13 | 5        | 0.17          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG21 | 10       | 0.17          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG22 | 10       | 0.17          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG23 | 10       | 0.17          |
| (1,1273) | 1:58:A:ASP:HA  | 1:59:A:ASN:HD21 | 3        | 0.17          |
| (1,1273) | 1:58:A:ASP:HA  | 1:59:A:ASN:HD22 | 3        | 0.17          |
| (1,1273) | 1:58:A:ASP:HA  | 1:59:A:ASN:HD21 | 5        | 0.17          |
| (1,1273) | 1:58:A:ASP:HA  | 1:59:A:ASN:HD22 | 5        | 0.17          |
| (1,1273) | 1:58:A:ASP:HA  | 1:59:A:ASN:HD21 | 6        | 0.17          |
| (1,1273) | 1:58:A:ASP:HA  | 1:59:A:ASN:HD22 | 6        | 0.17          |
| (1,1273) | 1:58:A:ASP:HA  | 1:59:A:ASN:HD21 | 14       | 0.17          |
| (1,1273) | 1:58:A:ASP:HA  | 1:59:A:ASN:HD22 | 14       | 0.17          |
| (1,1264) | 1:57:A:LYS:HG2 | 1:58:A:ASP:HA   | 13       | 0.17          |
| (1,1264) | 1:57:A:LYS:HG3 | 1:58:A:ASP:HA   | 13       | 0.17          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD2  | 3        | 0.17          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD3  | 3        | 0.17          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD2  | 4        | 0.17          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD3  | 4        | 0.17          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD2  | 12       | 0.17          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD3  | 12       | 0.17          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG2  | 18       | 0.17          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG3  | 18       | 0.17          |
| (1,1233) | 1:55:A:LEU:HG  | 1:63:A:ILE:HB   | 6        | 0.17          |
| (1,1233) | 1:55:A:LEU:HG  | 1:63:A:ILE:HB   | 7        | 0.17          |
| (1,1233) | 1:55:A:LEU:HG  | 1:63:A:ILE:HB   | 9        | 0.17          |
| (1,1168) | 1:52:A:HIS:HD2 | 1:52:A:HIS:HB2  | 9        | 0.17          |
| (1,1168) | 1:52:A:HIS:HD2 | 1:52:A:HIS:HB3  | 9        | 0.17          |
| (1,1168) | 1:52:A:HIS:HD2 | 1:52:A:HIS:HB2  | 10       | 0.17          |
| (1,1168) | 1:52:A:HIS:HD2 | 1:52:A:HIS:HB3  | 10       | 0.17          |
| (1,1168) | 1:52:A:HIS:HD2 | 1:52:A:HIS:HB2  | 15       | 0.17          |
| (1,1168) | 1:52:A:HIS:HD2 | 1:52:A:HIS:HB3  | 15       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1168) | 1:52:A:HIS:HD2  | 1:52:A:HIS:HB2  | 17       | 0.17          |
| (1,1168) | 1:52:A:HIS:HD2  | 1:52:A:HIS:HB3  | 17       | 0.17          |
| (1,1105) | 1:49:A:LEU:HB2  | 1:52:A:HIS:HD2  | 13       | 0.17          |
| (1,1105) | 1:49:A:LEU:HB3  | 1:52:A:HIS:HD2  | 13       | 0.17          |
| (1,1062) | 1:47:A:SER:HA   | 1:51:A:SER:H    | 13       | 0.17          |
| (1,1010) | 1:45:A:TRP:HE1  | 1:66:A:ILE:HG12 | 16       | 0.17          |
| (1,1010) | 1:45:A:TRP:HE1  | 1:66:A:ILE:HG13 | 16       | 0.17          |
| (1,997)  | 1:45:A:TRP:HA   | 1:50:A:GLU:H    | 13       | 0.17          |
| (1,918)  | 1:40:A:THR:HA   | 1:41:A:THR:H    | 10       | 0.17          |
| (1,894)  | 1:39:A:ILE:HD11 | 1:45:A:TRP:HH2  | 18       | 0.17          |
| (1,894)  | 1:39:A:ILE:HD12 | 1:45:A:TRP:HH2  | 18       | 0.17          |
| (1,894)  | 1:39:A:ILE:HD13 | 1:45:A:TRP:HH2  | 18       | 0.17          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG21 | 8        | 0.17          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG22 | 8        | 0.17          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG23 | 8        | 0.17          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG21 | 8        | 0.17          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG22 | 8        | 0.17          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG23 | 8        | 0.17          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG21 | 8        | 0.17          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG22 | 8        | 0.17          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG23 | 8        | 0.17          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG21 | 10       | 0.17          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG22 | 10       | 0.17          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG23 | 10       | 0.17          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG21 | 10       | 0.17          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG22 | 10       | 0.17          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG23 | 10       | 0.17          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG21 | 10       | 0.17          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG22 | 10       | 0.17          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG23 | 10       | 0.17          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG21 | 20       | 0.17          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG22 | 20       | 0.17          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG23 | 20       | 0.17          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG21 | 20       | 0.17          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG22 | 20       | 0.17          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG23 | 20       | 0.17          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG21 | 20       | 0.17          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG22 | 20       | 0.17          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG23 | 20       | 0.17          |
| (1,844)  | 1:37:A:GLU:H    | 1:38:A:GLU:H    | 7        | 0.17          |
| (1,844)  | 1:37:A:GLU:H    | 1:38:A:GLU:H    | 11       | 0.17          |
| (1,843)  | 1:37:A:GLU:HA   | 1:37:A:GLU:HG2  | 5        | 0.17          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,843) | 1:37:A:GLU:HA   | 1:37:A:GLU:HG3  | 5        | 0.17          |
| (1,792) | 1:34:A:GLU:HA   | 1:34:A:GLU:HG2  | 6        | 0.17          |
| (1,792) | 1:34:A:GLU:HA   | 1:34:A:GLU:HG3  | 6        | 0.17          |
| (1,772) | 1:31:A:ILE:HG21 | 1:49:A:LEU:HA   | 6        | 0.17          |
| (1,772) | 1:31:A:ILE:HG22 | 1:49:A:LEU:HA   | 6        | 0.17          |
| (1,772) | 1:31:A:ILE:HG23 | 1:49:A:LEU:HA   | 6        | 0.17          |
| (1,743) | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD2  | 3        | 0.17          |
| (1,743) | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD3  | 3        | 0.17          |
| (1,743) | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD2  | 3        | 0.17          |
| (1,743) | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD3  | 3        | 0.17          |
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD2  | 3        | 0.17          |
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD3  | 3        | 0.17          |
| (1,743) | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD2  | 20       | 0.17          |
| (1,743) | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD3  | 20       | 0.17          |
| (1,743) | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD2  | 20       | 0.17          |
| (1,743) | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD3  | 20       | 0.17          |
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD2  | 20       | 0.17          |
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD3  | 20       | 0.17          |
| (1,705) | 1:29:A:GLU:HA   | 1:29:A:GLU:HG2  | 7        | 0.17          |
| (1,705) | 1:29:A:GLU:HA   | 1:29:A:GLU:HG3  | 7        | 0.17          |
| (1,669) | 1:27:A:CYS:HB2  | 1:30:A:ASP:H    | 9        | 0.17          |
| (1,669) | 1:27:A:CYS:HB3  | 1:30:A:ASP:H    | 9        | 0.17          |
| (1,669) | 1:27:A:CYS:HB2  | 1:30:A:ASP:H    | 11       | 0.17          |
| (1,669) | 1:27:A:CYS:HB3  | 1:30:A:ASP:H    | 11       | 0.17          |
| (1,669) | 1:27:A:CYS:HB2  | 1:30:A:ASP:H    | 12       | 0.17          |
| (1,669) | 1:27:A:CYS:HB3  | 1:30:A:ASP:H    | 12       | 0.17          |
| (1,627) | 1:24:A:LYS:HG2  | 1:45:A:TRP:HD1  | 7        | 0.17          |
| (1,627) | 1:24:A:LYS:HG3  | 1:45:A:TRP:HD1  | 7        | 0.17          |
| (1,627) | 1:24:A:LYS:HG2  | 1:45:A:TRP:HD1  | 15       | 0.17          |
| (1,627) | 1:24:A:LYS:HG3  | 1:45:A:TRP:HD1  | 15       | 0.17          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG21 | 4        | 0.17          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG22 | 4        | 0.17          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG23 | 4        | 0.17          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG21 | 16       | 0.17          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG22 | 16       | 0.17          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG23 | 16       | 0.17          |
| (1,476) | 1:19:A:ASP:H    | 1:20:A:LEU:H    | 8        | 0.17          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB2  | 3        | 0.17          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB3  | 3        | 0.17          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB2  | 3        | 0.17          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB3  | 3        | 0.17          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB2  | 3        | 0.17          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB3  | 3        | 0.17          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB2  | 18       | 0.17          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB3  | 18       | 0.17          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB2  | 18       | 0.17          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB3  | 18       | 0.17          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB2  | 18       | 0.17          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB3  | 18       | 0.17          |
| (1,420) | 1:16:A:THR:HG21 | 1:17:A:LEU:H    | 2        | 0.17          |
| (1,420) | 1:16:A:THR:HG22 | 1:17:A:LEU:H    | 2        | 0.17          |
| (1,420) | 1:16:A:THR:HG23 | 1:17:A:LEU:H    | 2        | 0.17          |
| (1,420) | 1:16:A:THR:HG21 | 1:17:A:LEU:H    | 14       | 0.17          |
| (1,420) | 1:16:A:THR:HG22 | 1:17:A:LEU:H    | 14       | 0.17          |
| (1,420) | 1:16:A:THR:HG23 | 1:17:A:LEU:H    | 14       | 0.17          |
| (1,405) | 1:15:A:ILE:HD11 | 1:43:A:SER:H    | 1        | 0.17          |
| (1,405) | 1:15:A:ILE:HD12 | 1:43:A:SER:H    | 1        | 0.17          |
| (1,405) | 1:15:A:ILE:HD13 | 1:43:A:SER:H    | 1        | 0.17          |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE1  | 4        | 0.17          |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE2  | 4        | 0.17          |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE1  | 17       | 0.17          |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE2  | 17       | 0.17          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD1  | 7        | 0.17          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD2  | 7        | 0.17          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD1  | 7        | 0.17          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD2  | 7        | 0.17          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD1  | 7        | 0.17          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD2  | 7        | 0.17          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD1  | 9        | 0.17          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD2  | 9        | 0.17          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD1  | 9        | 0.17          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD2  | 9        | 0.17          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD1  | 9        | 0.17          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD2  | 9        | 0.17          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG21 | 6        | 0.17          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG22 | 6        | 0.17          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG23 | 6        | 0.17          |
| (1,245) | 1:9:A:GLN:HE22  | 1:12:A:THR:HG21 | 6        | 0.17          |
| (1,245) | 1:9:A:GLN:HE22  | 1:12:A:THR:HG22 | 6        | 0.17          |
| (1,245) | 1:9:A:GLN:HE22  | 1:12:A:THR:HG23 | 6        | 0.17          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG21 | 13       | 0.17          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG22 | 13       | 0.17          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG23 | 13       | 0.17          |
| (1,245) | 1:9:A:GLN:HE22  | 1:12:A:THR:HG21 | 13       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,245)  | 1:9:A:GLN:HE22  | 1:12:A:THR:HG22 | 13       | 0.17          |
| (1,245)  | 1:9:A:GLN:HE22  | 1:12:A:THR:HG23 | 13       | 0.17          |
| (1,245)  | 1:9:A:GLN:HE21  | 1:12:A:THR:HG21 | 19       | 0.17          |
| (1,245)  | 1:9:A:GLN:HE21  | 1:12:A:THR:HG22 | 19       | 0.17          |
| (1,245)  | 1:9:A:GLN:HE21  | 1:12:A:THR:HG23 | 19       | 0.17          |
| (1,245)  | 1:9:A:GLN:HE22  | 1:12:A:THR:HG21 | 19       | 0.17          |
| (1,245)  | 1:9:A:GLN:HE22  | 1:12:A:THR:HG22 | 19       | 0.17          |
| (1,245)  | 1:9:A:GLN:HE22  | 1:12:A:THR:HG23 | 19       | 0.17          |
| (1,127)  | 1:6:A:THR:HB    | 1:9:A:GLN:HG2   | 14       | 0.17          |
| (1,127)  | 1:6:A:THR:HB    | 1:9:A:GLN:HG3   | 14       | 0.17          |
| (1,124)  | 1:6:A:THR:HA    | 1:9:A:GLN:HG2   | 12       | 0.17          |
| (1,124)  | 1:6:A:THR:HA    | 1:9:A:GLN:HG3   | 12       | 0.17          |
| (1,124)  | 1:6:A:THR:HA    | 1:9:A:GLN:HG2   | 20       | 0.17          |
| (1,124)  | 1:6:A:THR:HA    | 1:9:A:GLN:HG3   | 20       | 0.17          |
| (1,112)  | 1:6:A:THR:HG21  | 1:6:A:THR:H     | 3        | 0.17          |
| (1,112)  | 1:6:A:THR:HG22  | 1:6:A:THR:H     | 3        | 0.17          |
| (1,112)  | 1:6:A:THR:HG23  | 1:6:A:THR:H     | 3        | 0.17          |
| (1,20)   | 1:2:A:ALA:HA    | 1:5:A:GLY:H     | 6        | 0.17          |
| (1,20)   | 1:2:A:ALA:HA    | 1:5:A:GLY:H     | 12       | 0.17          |
| (1,20)   | 1:2:A:ALA:HA    | 1:5:A:GLY:H     | 16       | 0.17          |
| (1,10)   | 1:1:A:MET:HA    | 1:57:A:LYS:HD2  | 2        | 0.17          |
| (1,10)   | 1:1:A:MET:HA    | 1:57:A:LYS:HD3  | 2        | 0.17          |
| (1,6)    | 1:1:A:MET:HA    | 1:3:A:GLU:H     | 14       | 0.17          |
| (1,1900) | 1:89:A:ILE:HG21 | 1:90:A:SER:HB2  | 14       | 0.16          |
| (1,1900) | 1:89:A:ILE:HG21 | 1:90:A:SER:HB3  | 14       | 0.16          |
| (1,1900) | 1:89:A:ILE:HG22 | 1:90:A:SER:HB2  | 14       | 0.16          |
| (1,1900) | 1:89:A:ILE:HG22 | 1:90:A:SER:HB3  | 14       | 0.16          |
| (1,1900) | 1:89:A:ILE:HG23 | 1:90:A:SER:HB2  | 14       | 0.16          |
| (1,1900) | 1:89:A:ILE:HG23 | 1:90:A:SER:HB3  | 14       | 0.16          |
| (1,1888) | 1:89:A:ILE:HG21 | 1:89:A:ILE:H    | 2        | 0.16          |
| (1,1888) | 1:89:A:ILE:HG22 | 1:89:A:ILE:H    | 2        | 0.16          |
| (1,1888) | 1:89:A:ILE:HG23 | 1:89:A:ILE:H    | 2        | 0.16          |
| (1,1888) | 1:89:A:ILE:HG21 | 1:89:A:ILE:H    | 12       | 0.16          |
| (1,1888) | 1:89:A:ILE:HG22 | 1:89:A:ILE:H    | 12       | 0.16          |
| (1,1888) | 1:89:A:ILE:HG23 | 1:89:A:ILE:H    | 12       | 0.16          |
| (1,1823) | 1:84:A:THR:HB   | 1:87:A:LEU:HB2  | 20       | 0.16          |
| (1,1823) | 1:84:A:THR:HB   | 1:87:A:LEU:HB3  | 20       | 0.16          |
| (1,1794) | 1:83:A:ARG:HG2  | 1:84:A:THR:H    | 2        | 0.16          |
| (1,1794) | 1:83:A:ARG:HG3  | 1:84:A:THR:H    | 2        | 0.16          |
| (1,1794) | 1:83:A:ARG:HG2  | 1:84:A:THR:H    | 5        | 0.16          |
| (1,1794) | 1:83:A:ARG:HG3  | 1:84:A:THR:H    | 5        | 0.16          |
| (1,1794) | 1:83:A:ARG:HG2  | 1:84:A:THR:H    | 18       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1794) | 1:83:A:ARG:HG3  | 1:84:A:THR:H    | 18       | 0.16          |
| (1,1777) | 1:82:A:TYR:HD1  | 1:85:A:ARG:HG2  | 1        | 0.16          |
| (1,1777) | 1:82:A:TYR:HD1  | 1:85:A:ARG:HG3  | 1        | 0.16          |
| (1,1777) | 1:82:A:TYR:HD2  | 1:85:A:ARG:HG2  | 1        | 0.16          |
| (1,1777) | 1:82:A:TYR:HD2  | 1:85:A:ARG:HG3  | 1        | 0.16          |
| (1,1777) | 1:82:A:TYR:HD1  | 1:85:A:ARG:HG2  | 4        | 0.16          |
| (1,1777) | 1:82:A:TYR:HD1  | 1:85:A:ARG:HG3  | 4        | 0.16          |
| (1,1777) | 1:82:A:TYR:HD2  | 1:85:A:ARG:HG2  | 4        | 0.16          |
| (1,1777) | 1:82:A:TYR:HD2  | 1:85:A:ARG:HG3  | 4        | 0.16          |
| (1,1762) | 1:82:A:TYR:HE1  | 1:82:A:TYR:H    | 10       | 0.16          |
| (1,1762) | 1:82:A:TYR:HE2  | 1:82:A:TYR:H    | 10       | 0.16          |
| (1,1762) | 1:82:A:TYR:HE1  | 1:82:A:TYR:H    | 13       | 0.16          |
| (1,1762) | 1:82:A:TYR:HE2  | 1:82:A:TYR:H    | 13       | 0.16          |
| (1,1762) | 1:82:A:TYR:HE1  | 1:82:A:TYR:H    | 18       | 0.16          |
| (1,1762) | 1:82:A:TYR:HE2  | 1:82:A:TYR:H    | 18       | 0.16          |
| (1,1669) | 1:76:A:LEU:HD11 | 1:80:A:VAL:HB   | 15       | 0.16          |
| (1,1669) | 1:76:A:LEU:HD12 | 1:80:A:VAL:HB   | 15       | 0.16          |
| (1,1669) | 1:76:A:LEU:HD13 | 1:80:A:VAL:HB   | 15       | 0.16          |
| (1,1669) | 1:76:A:LEU:HD21 | 1:80:A:VAL:HB   | 15       | 0.16          |
| (1,1669) | 1:76:A:LEU:HD22 | 1:80:A:VAL:HB   | 15       | 0.16          |
| (1,1669) | 1:76:A:LEU:HD23 | 1:80:A:VAL:HB   | 15       | 0.16          |
| (1,1669) | 1:76:A:LEU:HD11 | 1:80:A:VAL:HB   | 16       | 0.16          |
| (1,1669) | 1:76:A:LEU:HD12 | 1:80:A:VAL:HB   | 16       | 0.16          |
| (1,1669) | 1:76:A:LEU:HD13 | 1:80:A:VAL:HB   | 16       | 0.16          |
| (1,1669) | 1:76:A:LEU:HD21 | 1:80:A:VAL:HB   | 16       | 0.16          |
| (1,1669) | 1:76:A:LEU:HD22 | 1:80:A:VAL:HB   | 16       | 0.16          |
| (1,1669) | 1:76:A:LEU:HD23 | 1:80:A:VAL:HB   | 16       | 0.16          |
| (1,1669) | 1:76:A:LEU:HD11 | 1:80:A:VAL:HB   | 20       | 0.16          |
| (1,1669) | 1:76:A:LEU:HD12 | 1:80:A:VAL:HB   | 20       | 0.16          |
| (1,1669) | 1:76:A:LEU:HD13 | 1:80:A:VAL:HB   | 20       | 0.16          |
| (1,1669) | 1:76:A:LEU:HD21 | 1:80:A:VAL:HB   | 20       | 0.16          |
| (1,1669) | 1:76:A:LEU:HD22 | 1:80:A:VAL:HB   | 20       | 0.16          |
| (1,1669) | 1:76:A:LEU:HD23 | 1:80:A:VAL:HB   | 20       | 0.16          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG11 | 5        | 0.16          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG12 | 5        | 0.16          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG13 | 5        | 0.16          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG21 | 5        | 0.16          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG22 | 5        | 0.16          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG23 | 5        | 0.16          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG11 | 5        | 0.16          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG12 | 5        | 0.16          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG13 | 5        | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG21 | 5        | 0.16          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG22 | 5        | 0.16          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG23 | 5        | 0.16          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG11 | 16       | 0.16          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG12 | 16       | 0.16          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG13 | 16       | 0.16          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG21 | 16       | 0.16          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG22 | 16       | 0.16          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG23 | 16       | 0.16          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG11 | 16       | 0.16          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG12 | 16       | 0.16          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG13 | 16       | 0.16          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG21 | 16       | 0.16          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG22 | 16       | 0.16          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG23 | 16       | 0.16          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG11 | 19       | 0.16          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG12 | 19       | 0.16          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG13 | 19       | 0.16          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG21 | 19       | 0.16          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG22 | 19       | 0.16          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG23 | 19       | 0.16          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG11 | 19       | 0.16          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG12 | 19       | 0.16          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG13 | 19       | 0.16          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG21 | 19       | 0.16          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG22 | 19       | 0.16          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG23 | 19       | 0.16          |
| (1,1525) | 1:68:A:GLU:HA   | 1:68:A:GLU:HG2  | 6        | 0.16          |
| (1,1525) | 1:68:A:GLU:HA   | 1:68:A:GLU:HG3  | 6        | 0.16          |
| (1,1516) | 1:67:A:PHE:H    | 1:76:A:LEU:HG   | 10       | 0.16          |
| (1,1454) | 1:66:A:ILE:HA   | 1:67:A:PHE:H    | 10       | 0.16          |
| (1,1454) | 1:66:A:ILE:HA   | 1:67:A:PHE:H    | 18       | 0.16          |
| (1,1439) | 1:65:A:HIS:HA   | 1:69:A:ILE:H    | 7        | 0.16          |
| (1,1439) | 1:65:A:HIS:HA   | 1:69:A:ILE:H    | 13       | 0.16          |
| (1,1437) | 1:65:A:HIS:HA   | 1:68:A:GLU:H    | 2        | 0.16          |
| (1,1437) | 1:65:A:HIS:HA   | 1:68:A:GLU:H    | 5        | 0.16          |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG11 | 13       | 0.16          |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG12 | 13       | 0.16          |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG13 | 13       | 0.16          |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG21 | 13       | 0.16          |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG22 | 13       | 0.16          |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG23 | 13       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG11 | 13       | 0.16          |
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG12 | 13       | 0.16          |
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG13 | 13       | 0.16          |
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG21 | 13       | 0.16          |
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG22 | 13       | 0.16          |
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG23 | 13       | 0.16          |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG11 | 13       | 0.16          |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG12 | 13       | 0.16          |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG13 | 13       | 0.16          |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG21 | 13       | 0.16          |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG22 | 13       | 0.16          |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG23 | 13       | 0.16          |
| (1,1355) | 1:63:A:ILE:HB   | 1:63:A:ILE:H    | 1        | 0.16          |
| (1,1355) | 1:63:A:ILE:HB   | 1:63:A:ILE:H    | 5        | 0.16          |
| (1,1355) | 1:63:A:ILE:HB   | 1:63:A:ILE:H    | 6        | 0.16          |
| (1,1355) | 1:63:A:ILE:HB   | 1:63:A:ILE:H    | 10       | 0.16          |
| (1,1355) | 1:63:A:ILE:HB   | 1:63:A:ILE:H    | 11       | 0.16          |
| (1,1351) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HG12 | 10       | 0.16          |
| (1,1351) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HG13 | 10       | 0.16          |
| (1,1351) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HG12 | 10       | 0.16          |
| (1,1351) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HG13 | 10       | 0.16          |
| (1,1349) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HD11 | 1        | 0.16          |
| (1,1349) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HD12 | 1        | 0.16          |
| (1,1349) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HD13 | 1        | 0.16          |
| (1,1349) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HD11 | 1        | 0.16          |
| (1,1349) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HD12 | 1        | 0.16          |
| (1,1349) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HD13 | 1        | 0.16          |
| (1,1349) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HD11 | 2        | 0.16          |
| (1,1349) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HD12 | 2        | 0.16          |
| (1,1349) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HD13 | 2        | 0.16          |
| (1,1349) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HD11 | 2        | 0.16          |
| (1,1349) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HD12 | 2        | 0.16          |
| (1,1349) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HD13 | 2        | 0.16          |
| (1,1319) | 1:61:A:SER:HA   | 1:63:A:ILE:HG21 | 12       | 0.16          |
| (1,1319) | 1:61:A:SER:HA   | 1:63:A:ILE:HG22 | 12       | 0.16          |
| (1,1319) | 1:61:A:SER:HA   | 1:63:A:ILE:HG23 | 12       | 0.16          |
| (1,1292) | 1:60:A:LEU:HA   | 1:60:A:LEU:HD11 | 1        | 0.16          |
| (1,1292) | 1:60:A:LEU:HA   | 1:60:A:LEU:HD12 | 1        | 0.16          |
| (1,1292) | 1:60:A:LEU:HA   | 1:60:A:LEU:HD13 | 1        | 0.16          |
| (1,1292) | 1:60:A:LEU:HA   | 1:60:A:LEU:HD21 | 1        | 0.16          |
| (1,1292) | 1:60:A:LEU:HA   | 1:60:A:LEU:HD22 | 1        | 0.16          |
| (1,1292) | 1:60:A:LEU:HA   | 1:60:A:LEU:HD23 | 1        | 0.16          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD11 | 2        | 0.16          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD12 | 2        | 0.16          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD13 | 2        | 0.16          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD21 | 2        | 0.16          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD22 | 2        | 0.16          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD23 | 2        | 0.16          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD11 | 14       | 0.16          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD12 | 14       | 0.16          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD13 | 14       | 0.16          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD21 | 14       | 0.16          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD22 | 14       | 0.16          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD23 | 14       | 0.16          |
| (1,1267) | 1:57:A:LYS:HD2 | 1:59:A:ASN:H    | 8        | 0.16          |
| (1,1267) | 1:57:A:LYS:HD3 | 1:59:A:ASN:H    | 8        | 0.16          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD2  | 16       | 0.16          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD3  | 16       | 0.16          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG2  | 10       | 0.16          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG3  | 10       | 0.16          |
| (1,1246) | 1:56:A:ASP:H   | 1:59:A:ASN:H    | 9        | 0.16          |
| (1,1233) | 1:55:A:LEU:HG  | 1:63:A:ILE:HB   | 2        | 0.16          |
| (1,1233) | 1:55:A:LEU:HG  | 1:63:A:ILE:HB   | 11       | 0.16          |
| (1,1233) | 1:55:A:LEU:HG  | 1:63:A:ILE:HB   | 13       | 0.16          |
| (1,1233) | 1:55:A:LEU:HG  | 1:63:A:ILE:HB   | 14       | 0.16          |
| (1,1211) | 1:54:A:LYS:HB2 | 1:62:A:TYR:H    | 3        | 0.16          |
| (1,1211) | 1:54:A:LYS:HB3 | 1:62:A:TYR:H    | 3        | 0.16          |
| (1,1211) | 1:54:A:LYS:HB2 | 1:62:A:TYR:H    | 16       | 0.16          |
| (1,1211) | 1:54:A:LYS:HB3 | 1:62:A:TYR:H    | 16       | 0.16          |
| (1,1207) | 1:54:A:LYS:HG2 | 1:62:A:TYR:HE1  | 2        | 0.16          |
| (1,1207) | 1:54:A:LYS:HG2 | 1:62:A:TYR:HE2  | 2        | 0.16          |
| (1,1207) | 1:54:A:LYS:HG3 | 1:62:A:TYR:HE1  | 2        | 0.16          |
| (1,1207) | 1:54:A:LYS:HG3 | 1:62:A:TYR:HE2  | 2        | 0.16          |
| (1,1168) | 1:52:A:HIS:HD2 | 1:52:A:HIS:HB2  | 4        | 0.16          |
| (1,1168) | 1:52:A:HIS:HD2 | 1:52:A:HIS:HB3  | 4        | 0.16          |
| (1,1168) | 1:52:A:HIS:HD2 | 1:52:A:HIS:HB2  | 5        | 0.16          |
| (1,1168) | 1:52:A:HIS:HD2 | 1:52:A:HIS:HB3  | 5        | 0.16          |
| (1,1168) | 1:52:A:HIS:HD2 | 1:52:A:HIS:HB2  | 6        | 0.16          |
| (1,1168) | 1:52:A:HIS:HD2 | 1:52:A:HIS:HB3  | 6        | 0.16          |
| (1,1168) | 1:52:A:HIS:HD2 | 1:52:A:HIS:HB2  | 7        | 0.16          |
| (1,1168) | 1:52:A:HIS:HD2 | 1:52:A:HIS:HB3  | 7        | 0.16          |
| (1,1168) | 1:52:A:HIS:HD2 | 1:52:A:HIS:HB2  | 11       | 0.16          |
| (1,1168) | 1:52:A:HIS:HD2 | 1:52:A:HIS:HB3  | 11       | 0.16          |
| (1,1168) | 1:52:A:HIS:HD2 | 1:52:A:HIS:HB2  | 13       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1168) | 1:52:A:HIS:HD2  | 1:52:A:HIS:HB3  | 13       | 0.16          |
| (1,1105) | 1:49:A:LEU:HB2  | 1:52:A:HIS:HD2  | 7        | 0.16          |
| (1,1105) | 1:49:A:LEU:HB3  | 1:52:A:HIS:HD2  | 7        | 0.16          |
| (1,1018) | 1:46:A:PHE:HD1  | 1:46:A:PHE:H    | 10       | 0.16          |
| (1,1018) | 1:46:A:PHE:HD2  | 1:46:A:PHE:H    | 10       | 0.16          |
| (1,997)  | 1:45:A:TRP:HA   | 1:50:A:GLU:H    | 5        | 0.16          |
| (1,997)  | 1:45:A:TRP:HA   | 1:50:A:GLU:H    | 8        | 0.16          |
| (1,997)  | 1:45:A:TRP:HA   | 1:50:A:GLU:H    | 10       | 0.16          |
| (1,997)  | 1:45:A:TRP:HA   | 1:50:A:GLU:H    | 17       | 0.16          |
| (1,997)  | 1:45:A:TRP:HA   | 1:50:A:GLU:H    | 20       | 0.16          |
| (1,926)  | 1:41:A:THR:HB   | 1:42:A:GLY:H    | 15       | 0.16          |
| (1,901)  | 1:39:A:ILE:HG12 | 1:45:A:TRP:HD1  | 16       | 0.16          |
| (1,901)  | 1:39:A:ILE:HG13 | 1:45:A:TRP:HD1  | 16       | 0.16          |
| (1,846)  | 1:37:A:GLU:HA   | 1:38:A:GLU:H    | 2        | 0.16          |
| (1,846)  | 1:37:A:GLU:HA   | 1:38:A:GLU:H    | 6        | 0.16          |
| (1,846)  | 1:37:A:GLU:HA   | 1:38:A:GLU:H    | 11       | 0.16          |
| (1,844)  | 1:37:A:GLU:H    | 1:38:A:GLU:H    | 6        | 0.16          |
| (1,844)  | 1:37:A:GLU:H    | 1:38:A:GLU:H    | 8        | 0.16          |
| (1,772)  | 1:31:A:ILE:HG21 | 1:49:A:LEU:HA   | 4        | 0.16          |
| (1,772)  | 1:31:A:ILE:HG22 | 1:49:A:LEU:HA   | 4        | 0.16          |
| (1,772)  | 1:31:A:ILE:HG23 | 1:49:A:LEU:HA   | 4        | 0.16          |
| (1,772)  | 1:31:A:ILE:HG21 | 1:49:A:LEU:HA   | 12       | 0.16          |
| (1,772)  | 1:31:A:ILE:HG22 | 1:49:A:LEU:HA   | 12       | 0.16          |
| (1,772)  | 1:31:A:ILE:HG23 | 1:49:A:LEU:HA   | 12       | 0.16          |
| (1,761)  | 1:31:A:ILE:HD11 | 1:45:A:TRP:HD1  | 15       | 0.16          |
| (1,761)  | 1:31:A:ILE:HD12 | 1:45:A:TRP:HD1  | 15       | 0.16          |
| (1,761)  | 1:31:A:ILE:HD13 | 1:45:A:TRP:HD1  | 15       | 0.16          |
| (1,669)  | 1:27:A:CYS:HB2  | 1:30:A:ASP:H    | 6        | 0.16          |
| (1,669)  | 1:27:A:CYS:HB3  | 1:30:A:ASP:H    | 6        | 0.16          |
| (1,669)  | 1:27:A:CYS:HB2  | 1:30:A:ASP:H    | 7        | 0.16          |
| (1,669)  | 1:27:A:CYS:HB3  | 1:30:A:ASP:H    | 7        | 0.16          |
| (1,669)  | 1:27:A:CYS:HB2  | 1:30:A:ASP:H    | 8        | 0.16          |
| (1,669)  | 1:27:A:CYS:HB3  | 1:30:A:ASP:H    | 8        | 0.16          |
| (1,669)  | 1:27:A:CYS:HB2  | 1:30:A:ASP:H    | 18       | 0.16          |
| (1,669)  | 1:27:A:CYS:HB3  | 1:30:A:ASP:H    | 18       | 0.16          |
| (1,570)  | 1:22:A:GLN:H    | 1:66:A:ILE:HG21 | 17       | 0.16          |
| (1,570)  | 1:22:A:GLN:H    | 1:66:A:ILE:HG22 | 17       | 0.16          |
| (1,570)  | 1:22:A:GLN:H    | 1:66:A:ILE:HG23 | 17       | 0.16          |
| (1,557)  | 1:22:A:GLN:HE21 | 1:23:A:LEU:HA   | 14       | 0.16          |
| (1,557)  | 1:22:A:GLN:HE22 | 1:23:A:LEU:HA   | 14       | 0.16          |
| (1,534)  | 1:20:A:LEU:HD11 | 1:67:A:PHE:HE1  | 2        | 0.16          |
| (1,534)  | 1:20:A:LEU:HD11 | 1:67:A:PHE:HE2  | 2        | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,534) | 1:20:A:LEU:HD12 | 1:67:A:PHE:HE1  | 2        | 0.16          |
| (1,534) | 1:20:A:LEU:HD12 | 1:67:A:PHE:HE2  | 2        | 0.16          |
| (1,534) | 1:20:A:LEU:HD13 | 1:67:A:PHE:HE1  | 2        | 0.16          |
| (1,534) | 1:20:A:LEU:HD13 | 1:67:A:PHE:HE2  | 2        | 0.16          |
| (1,534) | 1:20:A:LEU:HD21 | 1:67:A:PHE:HE1  | 2        | 0.16          |
| (1,534) | 1:20:A:LEU:HD21 | 1:67:A:PHE:HE2  | 2        | 0.16          |
| (1,534) | 1:20:A:LEU:HD22 | 1:67:A:PHE:HE1  | 2        | 0.16          |
| (1,534) | 1:20:A:LEU:HD22 | 1:67:A:PHE:HE2  | 2        | 0.16          |
| (1,534) | 1:20:A:LEU:HD23 | 1:67:A:PHE:HE1  | 2        | 0.16          |
| (1,534) | 1:20:A:LEU:HD23 | 1:67:A:PHE:HE2  | 2        | 0.16          |
| (1,512) | 1:20:A:LEU:HB2  | 1:24:A:LYS:HG2  | 8        | 0.16          |
| (1,512) | 1:20:A:LEU:HB2  | 1:24:A:LYS:HG3  | 8        | 0.16          |
| (1,512) | 1:20:A:LEU:HB3  | 1:24:A:LYS:HG2  | 8        | 0.16          |
| (1,512) | 1:20:A:LEU:HB3  | 1:24:A:LYS:HG3  | 8        | 0.16          |
| (1,483) | 1:19:A:ASP:HA   | 1:22:A:GLN:HE21 | 13       | 0.16          |
| (1,483) | 1:19:A:ASP:HA   | 1:22:A:GLN:HE22 | 13       | 0.16          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB2  | 4        | 0.16          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB3  | 4        | 0.16          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB2  | 4        | 0.16          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB3  | 4        | 0.16          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB2  | 4        | 0.16          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB3  | 4        | 0.16          |
| (1,425) | 1:16:A:THR:HG21 | 1:18:A:GLU:H    | 17       | 0.16          |
| (1,425) | 1:16:A:THR:HG22 | 1:18:A:GLU:H    | 17       | 0.16          |
| (1,425) | 1:16:A:THR:HG23 | 1:18:A:GLU:H    | 17       | 0.16          |
| (1,420) | 1:16:A:THR:HG21 | 1:17:A:LEU:H    | 10       | 0.16          |
| (1,420) | 1:16:A:THR:HG22 | 1:17:A:LEU:H    | 10       | 0.16          |
| (1,420) | 1:16:A:THR:HG23 | 1:17:A:LEU:H    | 10       | 0.16          |
| (1,420) | 1:16:A:THR:HG21 | 1:17:A:LEU:H    | 18       | 0.16          |
| (1,420) | 1:16:A:THR:HG22 | 1:17:A:LEU:H    | 18       | 0.16          |
| (1,420) | 1:16:A:THR:HG23 | 1:17:A:LEU:H    | 18       | 0.16          |
| (1,405) | 1:15:A:ILE:HD11 | 1:43:A:SER:H    | 2        | 0.16          |
| (1,405) | 1:15:A:ILE:HD12 | 1:43:A:SER:H    | 2        | 0.16          |
| (1,405) | 1:15:A:ILE:HD13 | 1:43:A:SER:H    | 2        | 0.16          |
| (1,373) | 1:14:A:ASN:HB2  | 1:75:A:LEU:HG   | 4        | 0.16          |
| (1,373) | 1:14:A:ASN:HB3  | 1:75:A:LEU:HG   | 4        | 0.16          |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE1  | 1        | 0.16          |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE2  | 1        | 0.16          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD1  | 19       | 0.16          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD2  | 19       | 0.16          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD1  | 19       | 0.16          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD2  | 19       | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD1  | 19       | 0.16          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD2  | 19       | 0.16          |
| (1,335) | 1:12:A:THR:HB   | 1:42:A:GLY:H    | 8        | 0.16          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD11 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD12 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD13 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD21 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD22 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD23 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD11 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD12 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD13 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD21 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD22 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD23 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD11 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD12 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD13 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD21 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD22 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD23 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD11 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD12 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD13 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD21 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD22 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD23 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD11 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD12 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD13 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD21 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD22 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD23 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD11 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD12 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD13 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD21 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD22 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD23 | 2        | 0.16          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD11 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD12 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD13 | 6        | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD21 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD22 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD23 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD11 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD12 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD13 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD21 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD22 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD23 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD11 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD12 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD13 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD21 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD22 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD23 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD11 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD12 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD13 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD21 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD22 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD23 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD11 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD12 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD13 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD21 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD22 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD23 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD11 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD12 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD13 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD21 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD22 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD23 | 6        | 0.16          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD11 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD12 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD13 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD21 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD22 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD23 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD11 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD12 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD13 | 14       | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD21 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD22 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD23 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD11 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD12 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD13 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD21 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD22 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD23 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD11 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD12 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD13 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD21 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD22 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD23 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD11 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD12 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD13 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD21 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD22 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD23 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD11 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD12 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD13 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD21 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD22 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD23 | 14       | 0.16          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD11 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD12 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD13 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD21 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD22 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD23 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD11 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD12 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD13 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD21 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD22 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD23 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD11 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD12 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD13 | 17       | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD21 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD22 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD23 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD11 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD12 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD13 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD21 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD22 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD23 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD11 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD12 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD13 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD21 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD22 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD23 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD11 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD12 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD13 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD21 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD22 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD23 | 17       | 0.16          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD11 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD12 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD13 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD21 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD22 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD23 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD11 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD12 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD13 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD21 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD22 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD23 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD11 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD12 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD13 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD21 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD22 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD23 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD11 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD12 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD13 | 18       | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD21 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD22 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD23 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD11 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD12 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD13 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD21 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD22 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD23 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD11 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD12 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD13 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD21 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD22 | 18       | 0.16          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD23 | 18       | 0.16          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG21 | 2        | 0.16          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG22 | 2        | 0.16          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG23 | 2        | 0.16          |
| (1,245) | 1:9:A:GLN:HE22  | 1:12:A:THR:HG21 | 2        | 0.16          |
| (1,245) | 1:9:A:GLN:HE22  | 1:12:A:THR:HG22 | 2        | 0.16          |
| (1,245) | 1:9:A:GLN:HE22  | 1:12:A:THR:HG23 | 2        | 0.16          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG21 | 8        | 0.16          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG22 | 8        | 0.16          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG23 | 8        | 0.16          |
| (1,245) | 1:9:A:GLN:HE22  | 1:12:A:THR:HG21 | 8        | 0.16          |
| (1,245) | 1:9:A:GLN:HE22  | 1:12:A:THR:HG22 | 8        | 0.16          |
| (1,245) | 1:9:A:GLN:HE22  | 1:12:A:THR:HG23 | 8        | 0.16          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG21 | 15       | 0.16          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG22 | 15       | 0.16          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG23 | 15       | 0.16          |
| (1,245) | 1:9:A:GLN:HE22  | 1:12:A:THR:HG21 | 15       | 0.16          |
| (1,245) | 1:9:A:GLN:HE22  | 1:12:A:THR:HG22 | 15       | 0.16          |
| (1,245) | 1:9:A:GLN:HE22  | 1:12:A:THR:HG23 | 15       | 0.16          |
| (1,147) | 1:7:A:LEU:HG    | 1:8:A:LEU:HD11  | 10       | 0.16          |
| (1,147) | 1:7:A:LEU:HG    | 1:8:A:LEU:HD12  | 10       | 0.16          |
| (1,147) | 1:7:A:LEU:HG    | 1:8:A:LEU:HD13  | 10       | 0.16          |
| (1,147) | 1:7:A:LEU:HG    | 1:8:A:LEU:HD21  | 10       | 0.16          |
| (1,147) | 1:7:A:LEU:HG    | 1:8:A:LEU:HD22  | 10       | 0.16          |
| (1,147) | 1:7:A:LEU:HG    | 1:8:A:LEU:HD23  | 10       | 0.16          |
| (1,127) | 1:6:A:THR:HB    | 1:9:A:GLN:HG2   | 2        | 0.16          |
| (1,127) | 1:6:A:THR:HB    | 1:9:A:GLN:HG3   | 2        | 0.16          |
| (1,127) | 1:6:A:THR:HB    | 1:9:A:GLN:HG2   | 3        | 0.16          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,127)  | 1:6:A:THR:HB    | 1:9:A:GLN:HG3  | 3        | 0.16          |
| (1,127)  | 1:6:A:THR:HB    | 1:9:A:GLN:HG2  | 5        | 0.16          |
| (1,127)  | 1:6:A:THR:HB    | 1:9:A:GLN:HG3  | 5        | 0.16          |
| (1,127)  | 1:6:A:THR:HB    | 1:9:A:GLN:HG2  | 11       | 0.16          |
| (1,127)  | 1:6:A:THR:HB    | 1:9:A:GLN:HG3  | 11       | 0.16          |
| (1,112)  | 1:6:A:THR:HG21  | 1:6:A:THR:H    | 14       | 0.16          |
| (1,112)  | 1:6:A:THR:HG22  | 1:6:A:THR:H    | 14       | 0.16          |
| (1,112)  | 1:6:A:THR:HG23  | 1:6:A:THR:H    | 14       | 0.16          |
| (1,112)  | 1:6:A:THR:HG21  | 1:6:A:THR:H    | 19       | 0.16          |
| (1,112)  | 1:6:A:THR:HG22  | 1:6:A:THR:H    | 19       | 0.16          |
| (1,112)  | 1:6:A:THR:HG23  | 1:6:A:THR:H    | 19       | 0.16          |
| (1,93)   | 1:4:A:TYR:HA    | 1:82:A:TYR:HE1 | 4        | 0.16          |
| (1,93)   | 1:4:A:TYR:HA    | 1:82:A:TYR:HE2 | 4        | 0.16          |
| (1,80)   | 1:4:A:TYR:HD1   | 1:57:A:LYS:HB2 | 4        | 0.16          |
| (1,80)   | 1:4:A:TYR:HD1   | 1:57:A:LYS:HB3 | 4        | 0.16          |
| (1,80)   | 1:4:A:TYR:HD2   | 1:57:A:LYS:HB2 | 4        | 0.16          |
| (1,80)   | 1:4:A:TYR:HD2   | 1:57:A:LYS:HB3 | 4        | 0.16          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD11 | 3        | 0.16          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD12 | 3        | 0.16          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD13 | 3        | 0.16          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD21 | 3        | 0.16          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD22 | 3        | 0.16          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD23 | 3        | 0.16          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD11 | 3        | 0.16          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD12 | 3        | 0.16          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD13 | 3        | 0.16          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD21 | 3        | 0.16          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD22 | 3        | 0.16          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD23 | 3        | 0.16          |
| (1,20)   | 1:2:A:ALA:HA    | 1:5:A:GLY:H    | 4        | 0.16          |
| (1,20)   | 1:2:A:ALA:HA    | 1:5:A:GLY:H    | 8        | 0.16          |
| (1,20)   | 1:2:A:ALA:HA    | 1:5:A:GLY:H    | 9        | 0.16          |
| (1,20)   | 1:2:A:ALA:HA    | 1:5:A:GLY:H    | 11       | 0.16          |
| (1,20)   | 1:2:A:ALA:HA    | 1:5:A:GLY:H    | 15       | 0.16          |
| (1,1888) | 1:89:A:ILE:HG21 | 1:89:A:ILE:H   | 4        | 0.15          |
| (1,1888) | 1:89:A:ILE:HG22 | 1:89:A:ILE:H   | 4        | 0.15          |
| (1,1888) | 1:89:A:ILE:HG23 | 1:89:A:ILE:H   | 4        | 0.15          |
| (1,1888) | 1:89:A:ILE:HG21 | 1:89:A:ILE:H   | 13       | 0.15          |
| (1,1888) | 1:89:A:ILE:HG22 | 1:89:A:ILE:H   | 13       | 0.15          |
| (1,1888) | 1:89:A:ILE:HG23 | 1:89:A:ILE:H   | 13       | 0.15          |
| (1,1888) | 1:89:A:ILE:HG21 | 1:89:A:ILE:H   | 16       | 0.15          |
| (1,1888) | 1:89:A:ILE:HG22 | 1:89:A:ILE:H   | 16       | 0.15          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1888) | 1:89:A:ILE:HG23 | 1:89:A:ILE:H   | 16       | 0.15          |
| (1,1834) | 1:85:A:ARG:HD2  | 1:86:A:VAL:HA  | 12       | 0.15          |
| (1,1834) | 1:85:A:ARG:HD3  | 1:86:A:VAL:HA  | 12       | 0.15          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD2 | 2        | 0.15          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD3 | 2        | 0.15          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD2 | 2        | 0.15          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD3 | 2        | 0.15          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD2 | 2        | 0.15          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD3 | 2        | 0.15          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD2 | 14       | 0.15          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD3 | 14       | 0.15          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD2 | 14       | 0.15          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD3 | 14       | 0.15          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD2 | 14       | 0.15          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD3 | 14       | 0.15          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD2 | 16       | 0.15          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD3 | 16       | 0.15          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD2 | 16       | 0.15          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD3 | 16       | 0.15          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD2 | 16       | 0.15          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD3 | 16       | 0.15          |
| (1,1794) | 1:83:A:ARG:HG2  | 1:84:A:THR:H   | 14       | 0.15          |
| (1,1794) | 1:83:A:ARG:HG3  | 1:84:A:THR:H   | 14       | 0.15          |
| (1,1794) | 1:83:A:ARG:HG2  | 1:84:A:THR:H   | 20       | 0.15          |
| (1,1794) | 1:83:A:ARG:HG3  | 1:84:A:THR:H   | 20       | 0.15          |
| (1,1777) | 1:82:A:TYR:HD1  | 1:85:A:ARG:HG2 | 14       | 0.15          |
| (1,1777) | 1:82:A:TYR:HD1  | 1:85:A:ARG:HG3 | 14       | 0.15          |
| (1,1777) | 1:82:A:TYR:HD2  | 1:85:A:ARG:HG2 | 14       | 0.15          |
| (1,1777) | 1:82:A:TYR:HD2  | 1:85:A:ARG:HG3 | 14       | 0.15          |
| (1,1762) | 1:82:A:TYR:HE1  | 1:82:A:TYR:H   | 6        | 0.15          |
| (1,1762) | 1:82:A:TYR:HE2  | 1:82:A:TYR:H   | 6        | 0.15          |
| (1,1680) | 1:77:A:THR:HG21 | 1:78:A:MET:HG2 | 16       | 0.15          |
| (1,1680) | 1:77:A:THR:HG21 | 1:78:A:MET:HG3 | 16       | 0.15          |
| (1,1680) | 1:77:A:THR:HG22 | 1:78:A:MET:HG2 | 16       | 0.15          |
| (1,1680) | 1:77:A:THR:HG22 | 1:78:A:MET:HG3 | 16       | 0.15          |
| (1,1680) | 1:77:A:THR:HG23 | 1:78:A:MET:HG2 | 16       | 0.15          |
| (1,1680) | 1:77:A:THR:HG23 | 1:78:A:MET:HG3 | 16       | 0.15          |
| (1,1669) | 1:76:A:LEU:HD11 | 1:80:A:VAL:HB  | 4        | 0.15          |
| (1,1669) | 1:76:A:LEU:HD12 | 1:80:A:VAL:HB  | 4        | 0.15          |
| (1,1669) | 1:76:A:LEU:HD13 | 1:80:A:VAL:HB  | 4        | 0.15          |
| (1,1669) | 1:76:A:LEU:HD21 | 1:80:A:VAL:HB  | 4        | 0.15          |
| (1,1669) | 1:76:A:LEU:HD22 | 1:80:A:VAL:HB  | 4        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1669) | 1:76:A:LEU:HD23 | 1:80:A:VAL:HB   | 4        | 0.15          |
| (1,1669) | 1:76:A:LEU:HD11 | 1:80:A:VAL:HB   | 8        | 0.15          |
| (1,1669) | 1:76:A:LEU:HD12 | 1:80:A:VAL:HB   | 8        | 0.15          |
| (1,1669) | 1:76:A:LEU:HD13 | 1:80:A:VAL:HB   | 8        | 0.15          |
| (1,1669) | 1:76:A:LEU:HD21 | 1:80:A:VAL:HB   | 8        | 0.15          |
| (1,1669) | 1:76:A:LEU:HD22 | 1:80:A:VAL:HB   | 8        | 0.15          |
| (1,1669) | 1:76:A:LEU:HD23 | 1:80:A:VAL:HB   | 8        | 0.15          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG11 | 3        | 0.15          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG12 | 3        | 0.15          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG13 | 3        | 0.15          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG21 | 3        | 0.15          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG22 | 3        | 0.15          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG23 | 3        | 0.15          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG11 | 3        | 0.15          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG12 | 3        | 0.15          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG13 | 3        | 0.15          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG21 | 3        | 0.15          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG22 | 3        | 0.15          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG23 | 3        | 0.15          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG11 | 15       | 0.15          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG12 | 15       | 0.15          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG13 | 15       | 0.15          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG21 | 15       | 0.15          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG22 | 15       | 0.15          |
| (1,1666) | 1:76:A:LEU:HB2  | 1:80:A:VAL:HG23 | 15       | 0.15          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG11 | 15       | 0.15          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG12 | 15       | 0.15          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG13 | 15       | 0.15          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG21 | 15       | 0.15          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG22 | 15       | 0.15          |
| (1,1666) | 1:76:A:LEU:HB3  | 1:80:A:VAL:HG23 | 15       | 0.15          |
| (1,1609) | 1:73:A:PRO:HA   | 1:73:A:PRO:HG2  | 2        | 0.15          |
| (1,1609) | 1:73:A:PRO:HA   | 1:73:A:PRO:HG3  | 2        | 0.15          |
| (1,1609) | 1:73:A:PRO:HA   | 1:73:A:PRO:HG2  | 4        | 0.15          |
| (1,1609) | 1:73:A:PRO:HA   | 1:73:A:PRO:HG3  | 4        | 0.15          |
| (1,1609) | 1:73:A:PRO:HA   | 1:73:A:PRO:HG2  | 5        | 0.15          |
| (1,1609) | 1:73:A:PRO:HA   | 1:73:A:PRO:HG3  | 5        | 0.15          |
| (1,1597) | 1:72:A:ARG:HG2  | 1:74:A:ASP:H    | 14       | 0.15          |
| (1,1597) | 1:72:A:ARG:HG3  | 1:74:A:ASP:H    | 14       | 0.15          |
| (1,1541) | 1:68:A:GLU:HG2  | 1:76:A:LEU:HD11 | 6        | 0.15          |
| (1,1541) | 1:68:A:GLU:HG2  | 1:76:A:LEU:HD12 | 6        | 0.15          |
| (1,1541) | 1:68:A:GLU:HG2  | 1:76:A:LEU:HD13 | 6        | 0.15          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1541) | 1:68:A:GLU:HG2 | 1:76:A:LEU:HD21 | 6        | 0.15          |
| (1,1541) | 1:68:A:GLU:HG2 | 1:76:A:LEU:HD22 | 6        | 0.15          |
| (1,1541) | 1:68:A:GLU:HG2 | 1:76:A:LEU:HD23 | 6        | 0.15          |
| (1,1541) | 1:68:A:GLU:HG3 | 1:76:A:LEU:HD11 | 6        | 0.15          |
| (1,1541) | 1:68:A:GLU:HG3 | 1:76:A:LEU:HD12 | 6        | 0.15          |
| (1,1541) | 1:68:A:GLU:HG3 | 1:76:A:LEU:HD13 | 6        | 0.15          |
| (1,1541) | 1:68:A:GLU:HG3 | 1:76:A:LEU:HD21 | 6        | 0.15          |
| (1,1541) | 1:68:A:GLU:HG3 | 1:76:A:LEU:HD22 | 6        | 0.15          |
| (1,1541) | 1:68:A:GLU:HG3 | 1:76:A:LEU:HD23 | 6        | 0.15          |
| (1,1525) | 1:68:A:GLU:HA  | 1:68:A:GLU:HG2  | 19       | 0.15          |
| (1,1525) | 1:68:A:GLU:HA  | 1:68:A:GLU:HG3  | 19       | 0.15          |
| (1,1516) | 1:67:A:PHE:H   | 1:76:A:LEU:HG   | 18       | 0.15          |
| (1,1454) | 1:66:A:ILE:HA  | 1:67:A:PHE:H    | 4        | 0.15          |
| (1,1454) | 1:66:A:ILE:HA  | 1:67:A:PHE:H    | 11       | 0.15          |
| (1,1454) | 1:66:A:ILE:HA  | 1:67:A:PHE:H    | 16       | 0.15          |
| (1,1454) | 1:66:A:ILE:HA  | 1:67:A:PHE:H    | 20       | 0.15          |
| (1,1439) | 1:65:A:HIS:HA  | 1:69:A:ILE:H    | 5        | 0.15          |
| (1,1439) | 1:65:A:HIS:HA  | 1:69:A:ILE:H    | 8        | 0.15          |
| (1,1439) | 1:65:A:HIS:HA  | 1:69:A:ILE:H    | 11       | 0.15          |
| (1,1437) | 1:65:A:HIS:HA  | 1:68:A:GLU:H    | 1        | 0.15          |
| (1,1437) | 1:65:A:HIS:HA  | 1:68:A:GLU:H    | 17       | 0.15          |
| (1,1437) | 1:65:A:HIS:HA  | 1:68:A:GLU:H    | 20       | 0.15          |
| (1,1428) | 1:65:A:HIS:HD2 | 1:66:A:ILE:HG12 | 1        | 0.15          |
| (1,1428) | 1:65:A:HIS:HD2 | 1:66:A:ILE:HG13 | 1        | 0.15          |
| (1,1428) | 1:65:A:HIS:HD2 | 1:66:A:ILE:HG12 | 12       | 0.15          |
| (1,1428) | 1:65:A:HIS:HD2 | 1:66:A:ILE:HG13 | 12       | 0.15          |
| (1,1428) | 1:65:A:HIS:HD2 | 1:66:A:ILE:HG12 | 14       | 0.15          |
| (1,1428) | 1:65:A:HIS:HD2 | 1:66:A:ILE:HG13 | 14       | 0.15          |
| (1,1355) | 1:63:A:ILE:HB  | 1:63:A:ILE:H    | 2        | 0.15          |
| (1,1355) | 1:63:A:ILE:HB  | 1:63:A:ILE:H    | 16       | 0.15          |
| (1,1355) | 1:63:A:ILE:HB  | 1:63:A:ILE:H    | 17       | 0.15          |
| (1,1355) | 1:63:A:ILE:HB  | 1:63:A:ILE:H    | 19       | 0.15          |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG12 | 1        | 0.15          |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG13 | 1        | 0.15          |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG12 | 1        | 0.15          |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG13 | 1        | 0.15          |
| (1,1349) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HD11 | 15       | 0.15          |
| (1,1349) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HD12 | 15       | 0.15          |
| (1,1349) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HD13 | 15       | 0.15          |
| (1,1349) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HD11 | 15       | 0.15          |
| (1,1349) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HD12 | 15       | 0.15          |
| (1,1349) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HD13 | 15       | 0.15          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG21 | 20       | 0.15          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG22 | 20       | 0.15          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG23 | 20       | 0.15          |
| (1,1267) | 1:57:A:LYS:HD2 | 1:59:A:ASN:H    | 7        | 0.15          |
| (1,1267) | 1:57:A:LYS:HD3 | 1:59:A:ASN:H    | 7        | 0.15          |
| (1,1267) | 1:57:A:LYS:HD2 | 1:59:A:ASN:H    | 14       | 0.15          |
| (1,1267) | 1:57:A:LYS:HD3 | 1:59:A:ASN:H    | 14       | 0.15          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD2  | 8        | 0.15          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD3  | 8        | 0.15          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG2  | 1        | 0.15          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG3  | 1        | 0.15          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG2  | 7        | 0.15          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG3  | 7        | 0.15          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG2  | 15       | 0.15          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG3  | 15       | 0.15          |
| (1,1252) | 1:56:A:ASP:HB2 | 1:59:A:ASN:HD21 | 6        | 0.15          |
| (1,1252) | 1:56:A:ASP:HB2 | 1:59:A:ASN:HD22 | 6        | 0.15          |
| (1,1252) | 1:56:A:ASP:HB3 | 1:59:A:ASN:HD21 | 6        | 0.15          |
| (1,1252) | 1:56:A:ASP:HB3 | 1:59:A:ASN:HD22 | 6        | 0.15          |
| (1,1251) | 1:56:A:ASP:H   | 1:59:A:ASN:HD21 | 9        | 0.15          |
| (1,1251) | 1:56:A:ASP:H   | 1:59:A:ASN:HD22 | 9        | 0.15          |
| (1,1233) | 1:55:A:LEU:HG  | 1:63:A:ILE:HB   | 3        | 0.15          |
| (1,1233) | 1:55:A:LEU:HG  | 1:63:A:ILE:HB   | 5        | 0.15          |
| (1,1233) | 1:55:A:LEU:HG  | 1:63:A:ILE:HB   | 10       | 0.15          |
| (1,1228) | 1:55:A:LEU:HG  | 1:59:A:ASN:HD21 | 3        | 0.15          |
| (1,1228) | 1:55:A:LEU:HG  | 1:59:A:ASN:HD22 | 3        | 0.15          |
| (1,1228) | 1:55:A:LEU:HG  | 1:59:A:ASN:HD21 | 7        | 0.15          |
| (1,1228) | 1:55:A:LEU:HG  | 1:59:A:ASN:HD22 | 7        | 0.15          |
| (1,1223) | 1:55:A:LEU:HG  | 1:56:A:ASP:HA   | 9        | 0.15          |
| (1,1211) | 1:54:A:LYS:HB2 | 1:62:A:TYR:H    | 13       | 0.15          |
| (1,1211) | 1:54:A:LYS:HB3 | 1:62:A:TYR:H    | 13       | 0.15          |
| (1,1207) | 1:54:A:LYS:HG2 | 1:62:A:TYR:HE1  | 12       | 0.15          |
| (1,1207) | 1:54:A:LYS:HG2 | 1:62:A:TYR:HE2  | 12       | 0.15          |
| (1,1207) | 1:54:A:LYS:HG3 | 1:62:A:TYR:HE1  | 12       | 0.15          |
| (1,1207) | 1:54:A:LYS:HG3 | 1:62:A:TYR:HE2  | 12       | 0.15          |
| (1,1207) | 1:54:A:LYS:HG2 | 1:62:A:TYR:HE1  | 19       | 0.15          |
| (1,1207) | 1:54:A:LYS:HG2 | 1:62:A:TYR:HE2  | 19       | 0.15          |
| (1,1207) | 1:54:A:LYS:HG3 | 1:62:A:TYR:HE1  | 19       | 0.15          |
| (1,1207) | 1:54:A:LYS:HG3 | 1:62:A:TYR:HE2  | 19       | 0.15          |
| (1,1206) | 1:54:A:LYS:HB2 | 1:62:A:TYR:HE1  | 2        | 0.15          |
| (1,1206) | 1:54:A:LYS:HB2 | 1:62:A:TYR:HE2  | 2        | 0.15          |
| (1,1206) | 1:54:A:LYS:HB3 | 1:62:A:TYR:HE1  | 2        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1206) | 1:54:A:LYS:HB3  | 1:62:A:TYR:HE2  | 2        | 0.15          |
| (1,1168) | 1:52:A:HIS:HD2  | 1:52:A:HIS:HB2  | 2        | 0.15          |
| (1,1168) | 1:52:A:HIS:HD2  | 1:52:A:HIS:HB3  | 2        | 0.15          |
| (1,1168) | 1:52:A:HIS:HD2  | 1:52:A:HIS:HB2  | 12       | 0.15          |
| (1,1168) | 1:52:A:HIS:HD2  | 1:52:A:HIS:HB3  | 12       | 0.15          |
| (1,1062) | 1:47:A:SER:HA   | 1:51:A:SER:H    | 15       | 0.15          |
| (1,1062) | 1:47:A:SER:HA   | 1:51:A:SER:H    | 16       | 0.15          |
| (1,1018) | 1:46:A:PHE:HD1  | 1:46:A:PHE:H    | 16       | 0.15          |
| (1,1018) | 1:46:A:PHE:HD2  | 1:46:A:PHE:H    | 16       | 0.15          |
| (1,997)  | 1:45:A:TRP:HA   | 1:50:A:GLU:H    | 2        | 0.15          |
| (1,997)  | 1:45:A:TRP:HA   | 1:50:A:GLU:H    | 3        | 0.15          |
| (1,997)  | 1:45:A:TRP:HA   | 1:50:A:GLU:H    | 4        | 0.15          |
| (1,997)  | 1:45:A:TRP:HA   | 1:50:A:GLU:H    | 16       | 0.15          |
| (1,982)  | 1:45:A:TRP:HE1  | 1:46:A:PHE:HA   | 13       | 0.15          |
| (1,982)  | 1:45:A:TRP:HE1  | 1:46:A:PHE:HA   | 17       | 0.15          |
| (1,926)  | 1:41:A:THR:HB   | 1:42:A:GLY:H    | 20       | 0.15          |
| (1,894)  | 1:39:A:ILE:HD11 | 1:45:A:TRP:HH2  | 10       | 0.15          |
| (1,894)  | 1:39:A:ILE:HD12 | 1:45:A:TRP:HH2  | 10       | 0.15          |
| (1,894)  | 1:39:A:ILE:HD13 | 1:45:A:TRP:HH2  | 10       | 0.15          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG21 | 4        | 0.15          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG22 | 4        | 0.15          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG23 | 4        | 0.15          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG21 | 4        | 0.15          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG22 | 4        | 0.15          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG23 | 4        | 0.15          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG21 | 4        | 0.15          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG22 | 4        | 0.15          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG23 | 4        | 0.15          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG21 | 5        | 0.15          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG22 | 5        | 0.15          |
| (1,876)  | 1:39:A:ILE:HD11 | 1:40:A:THR:HG23 | 5        | 0.15          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG21 | 5        | 0.15          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG22 | 5        | 0.15          |
| (1,876)  | 1:39:A:ILE:HD12 | 1:40:A:THR:HG23 | 5        | 0.15          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG21 | 5        | 0.15          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG22 | 5        | 0.15          |
| (1,876)  | 1:39:A:ILE:HD13 | 1:40:A:THR:HG23 | 5        | 0.15          |
| (1,855)  | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD11 | 4        | 0.15          |
| (1,855)  | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD12 | 4        | 0.15          |
| (1,855)  | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD13 | 4        | 0.15          |
| (1,855)  | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD11 | 4        | 0.15          |
| (1,855)  | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD12 | 4        | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,855) | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD13 | 4        | 0.15          |
| (1,855) | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD11 | 19       | 0.15          |
| (1,855) | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD12 | 19       | 0.15          |
| (1,855) | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD13 | 19       | 0.15          |
| (1,855) | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD11 | 19       | 0.15          |
| (1,855) | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD12 | 19       | 0.15          |
| (1,855) | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD13 | 19       | 0.15          |
| (1,855) | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD11 | 20       | 0.15          |
| (1,855) | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD12 | 20       | 0.15          |
| (1,855) | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD13 | 20       | 0.15          |
| (1,855) | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD11 | 20       | 0.15          |
| (1,855) | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD12 | 20       | 0.15          |
| (1,855) | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD13 | 20       | 0.15          |
| (1,783) | 1:32:A:PRO:HD2  | 1:35:A:LYS:HG2  | 4        | 0.15          |
| (1,783) | 1:32:A:PRO:HD2  | 1:35:A:LYS:HG3  | 4        | 0.15          |
| (1,783) | 1:32:A:PRO:HD3  | 1:35:A:LYS:HG2  | 4        | 0.15          |
| (1,783) | 1:32:A:PRO:HD3  | 1:35:A:LYS:HG3  | 4        | 0.15          |
| (1,772) | 1:31:A:ILE:HG21 | 1:49:A:LEU:HA   | 1        | 0.15          |
| (1,772) | 1:31:A:ILE:HG22 | 1:49:A:LEU:HA   | 1        | 0.15          |
| (1,772) | 1:31:A:ILE:HG23 | 1:49:A:LEU:HA   | 1        | 0.15          |
| (1,772) | 1:31:A:ILE:HG21 | 1:49:A:LEU:HA   | 2        | 0.15          |
| (1,772) | 1:31:A:ILE:HG22 | 1:49:A:LEU:HA   | 2        | 0.15          |
| (1,772) | 1:31:A:ILE:HG23 | 1:49:A:LEU:HA   | 2        | 0.15          |
| (1,772) | 1:31:A:ILE:HG21 | 1:49:A:LEU:HA   | 3        | 0.15          |
| (1,772) | 1:31:A:ILE:HG22 | 1:49:A:LEU:HA   | 3        | 0.15          |
| (1,772) | 1:31:A:ILE:HG23 | 1:49:A:LEU:HA   | 3        | 0.15          |
| (1,736) | 1:31:A:ILE:HB   | 1:32:A:PRO:HA   | 7        | 0.15          |
| (1,736) | 1:31:A:ILE:HB   | 1:32:A:PRO:HA   | 14       | 0.15          |
| (1,724) | 1:31:A:ILE:HD11 | 1:31:A:ILE:H    | 17       | 0.15          |
| (1,724) | 1:31:A:ILE:HD12 | 1:31:A:ILE:H    | 17       | 0.15          |
| (1,724) | 1:31:A:ILE:HD13 | 1:31:A:ILE:H    | 17       | 0.15          |
| (1,669) | 1:27:A:CYS:HB2  | 1:30:A:ASP:H    | 2        | 0.15          |
| (1,669) | 1:27:A:CYS:HB3  | 1:30:A:ASP:H    | 2        | 0.15          |
| (1,669) | 1:27:A:CYS:HB2  | 1:30:A:ASP:H    | 4        | 0.15          |
| (1,669) | 1:27:A:CYS:HB3  | 1:30:A:ASP:H    | 4        | 0.15          |
| (1,669) | 1:27:A:CYS:HB2  | 1:30:A:ASP:H    | 14       | 0.15          |
| (1,669) | 1:27:A:CYS:HB3  | 1:30:A:ASP:H    | 14       | 0.15          |
| (1,627) | 1:24:A:LYS:HG2  | 1:45:A:TRP:HD1  | 3        | 0.15          |
| (1,627) | 1:24:A:LYS:HG3  | 1:45:A:TRP:HD1  | 3        | 0.15          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG21 | 10       | 0.15          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG22 | 10       | 0.15          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG23 | 10       | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG21 | 16       | 0.15          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG22 | 16       | 0.15          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG23 | 16       | 0.15          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG21 | 13       | 0.15          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG22 | 13       | 0.15          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG23 | 13       | 0.15          |
| (1,566) | 1:22:A:GLN:HG2  | 1:25:A:SER:HB2  | 9        | 0.15          |
| (1,566) | 1:22:A:GLN:HG2  | 1:25:A:SER:HB3  | 9        | 0.15          |
| (1,566) | 1:22:A:GLN:HG3  | 1:25:A:SER:HB2  | 9        | 0.15          |
| (1,566) | 1:22:A:GLN:HG3  | 1:25:A:SER:HB3  | 9        | 0.15          |
| (1,566) | 1:22:A:GLN:HG2  | 1:25:A:SER:HB2  | 11       | 0.15          |
| (1,566) | 1:22:A:GLN:HG2  | 1:25:A:SER:HB3  | 11       | 0.15          |
| (1,566) | 1:22:A:GLN:HG3  | 1:25:A:SER:HB2  | 11       | 0.15          |
| (1,566) | 1:22:A:GLN:HG3  | 1:25:A:SER:HB3  | 11       | 0.15          |
| (1,555) | 1:22:A:GLN:HA   | 1:23:A:LEU:H    | 2        | 0.15          |
| (1,555) | 1:22:A:GLN:HA   | 1:23:A:LEU:H    | 11       | 0.15          |
| (1,516) | 1:20:A:LEU:HD11 | 1:39:A:ILE:HD11 | 10       | 0.15          |
| (1,516) | 1:20:A:LEU:HD11 | 1:39:A:ILE:HD12 | 10       | 0.15          |
| (1,516) | 1:20:A:LEU:HD11 | 1:39:A:ILE:HD13 | 10       | 0.15          |
| (1,516) | 1:20:A:LEU:HD12 | 1:39:A:ILE:HD11 | 10       | 0.15          |
| (1,516) | 1:20:A:LEU:HD12 | 1:39:A:ILE:HD12 | 10       | 0.15          |
| (1,516) | 1:20:A:LEU:HD12 | 1:39:A:ILE:HD13 | 10       | 0.15          |
| (1,516) | 1:20:A:LEU:HD13 | 1:39:A:ILE:HD11 | 10       | 0.15          |
| (1,516) | 1:20:A:LEU:HD13 | 1:39:A:ILE:HD12 | 10       | 0.15          |
| (1,516) | 1:20:A:LEU:HD13 | 1:39:A:ILE:HD13 | 10       | 0.15          |
| (1,516) | 1:20:A:LEU:HD21 | 1:39:A:ILE:HD11 | 10       | 0.15          |
| (1,516) | 1:20:A:LEU:HD21 | 1:39:A:ILE:HD12 | 10       | 0.15          |
| (1,516) | 1:20:A:LEU:HD21 | 1:39:A:ILE:HD13 | 10       | 0.15          |
| (1,516) | 1:20:A:LEU:HD22 | 1:39:A:ILE:HD11 | 10       | 0.15          |
| (1,516) | 1:20:A:LEU:HD22 | 1:39:A:ILE:HD12 | 10       | 0.15          |
| (1,516) | 1:20:A:LEU:HD22 | 1:39:A:ILE:HD13 | 10       | 0.15          |
| (1,516) | 1:20:A:LEU:HD23 | 1:39:A:ILE:HD11 | 10       | 0.15          |
| (1,516) | 1:20:A:LEU:HD23 | 1:39:A:ILE:HD12 | 10       | 0.15          |
| (1,516) | 1:20:A:LEU:HD23 | 1:39:A:ILE:HD13 | 10       | 0.15          |
| (1,483) | 1:19:A:ASP:HA   | 1:22:A:GLN:HE21 | 6        | 0.15          |
| (1,483) | 1:19:A:ASP:HA   | 1:22:A:GLN:HE22 | 6        | 0.15          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB2  | 12       | 0.15          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB3  | 12       | 0.15          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB2  | 12       | 0.15          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB3  | 12       | 0.15          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB2  | 12       | 0.15          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB3  | 12       | 0.15          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB2 | 14       | 0.15          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB3 | 14       | 0.15          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB2 | 14       | 0.15          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB3 | 14       | 0.15          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB2 | 14       | 0.15          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB3 | 14       | 0.15          |
| (1,425) | 1:16:A:THR:HG21 | 1:18:A:GLU:H   | 3        | 0.15          |
| (1,425) | 1:16:A:THR:HG22 | 1:18:A:GLU:H   | 3        | 0.15          |
| (1,425) | 1:16:A:THR:HG23 | 1:18:A:GLU:H   | 3        | 0.15          |
| (1,425) | 1:16:A:THR:HG21 | 1:18:A:GLU:H   | 6        | 0.15          |
| (1,425) | 1:16:A:THR:HG22 | 1:18:A:GLU:H   | 6        | 0.15          |
| (1,425) | 1:16:A:THR:HG23 | 1:18:A:GLU:H   | 6        | 0.15          |
| (1,425) | 1:16:A:THR:HG21 | 1:18:A:GLU:H   | 9        | 0.15          |
| (1,425) | 1:16:A:THR:HG22 | 1:18:A:GLU:H   | 9        | 0.15          |
| (1,425) | 1:16:A:THR:HG23 | 1:18:A:GLU:H   | 9        | 0.15          |
| (1,425) | 1:16:A:THR:HG21 | 1:18:A:GLU:H   | 19       | 0.15          |
| (1,425) | 1:16:A:THR:HG22 | 1:18:A:GLU:H   | 19       | 0.15          |
| (1,425) | 1:16:A:THR:HG23 | 1:18:A:GLU:H   | 19       | 0.15          |
| (1,425) | 1:16:A:THR:HG21 | 1:18:A:GLU:H   | 20       | 0.15          |
| (1,425) | 1:16:A:THR:HG22 | 1:18:A:GLU:H   | 20       | 0.15          |
| (1,425) | 1:16:A:THR:HG23 | 1:18:A:GLU:H   | 20       | 0.15          |
| (1,420) | 1:16:A:THR:HG21 | 1:17:A:LEU:H   | 9        | 0.15          |
| (1,420) | 1:16:A:THR:HG22 | 1:17:A:LEU:H   | 9        | 0.15          |
| (1,420) | 1:16:A:THR:HG23 | 1:17:A:LEU:H   | 9        | 0.15          |
| (1,405) | 1:15:A:ILE:HD11 | 1:43:A:SER:H   | 8        | 0.15          |
| (1,405) | 1:15:A:ILE:HD12 | 1:43:A:SER:H   | 8        | 0.15          |
| (1,405) | 1:15:A:ILE:HD13 | 1:43:A:SER:H   | 8        | 0.15          |
| (1,387) | 1:15:A:ILE:HD11 | 1:19:A:ASP:H   | 7        | 0.15          |
| (1,387) | 1:15:A:ILE:HD12 | 1:19:A:ASP:H   | 7        | 0.15          |
| (1,387) | 1:15:A:ILE:HD13 | 1:19:A:ASP:H   | 7        | 0.15          |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE1 | 5        | 0.15          |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE2 | 5        | 0.15          |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE1 | 13       | 0.15          |
| (1,341) | 1:12:A:THR:H    | 1:46:A:PHE:HE2 | 13       | 0.15          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD1 | 2        | 0.15          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD2 | 2        | 0.15          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD1 | 2        | 0.15          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD2 | 2        | 0.15          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD1 | 2        | 0.15          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD2 | 2        | 0.15          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD1 | 5        | 0.15          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD2 | 5        | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD1  | 5        | 0.15          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD2  | 5        | 0.15          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD1  | 5        | 0.15          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD2  | 5        | 0.15          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG21 | 4        | 0.15          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG22 | 4        | 0.15          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG23 | 4        | 0.15          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG21 | 4        | 0.15          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG22 | 4        | 0.15          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG23 | 4        | 0.15          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG21 | 8        | 0.15          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG22 | 8        | 0.15          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG23 | 8        | 0.15          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG21 | 8        | 0.15          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG22 | 8        | 0.15          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG23 | 8        | 0.15          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG21 | 10       | 0.15          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG22 | 10       | 0.15          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG23 | 10       | 0.15          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG21 | 10       | 0.15          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG22 | 10       | 0.15          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG23 | 10       | 0.15          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG21 | 17       | 0.15          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG22 | 17       | 0.15          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG23 | 17       | 0.15          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG21 | 17       | 0.15          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG22 | 17       | 0.15          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG23 | 17       | 0.15          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG21 | 3        | 0.15          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG22 | 3        | 0.15          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG23 | 3        | 0.15          |
| (1,245) | 1:9:A:GLN:HE22  | 1:12:A:THR:HG21 | 3        | 0.15          |
| (1,245) | 1:9:A:GLN:HE22  | 1:12:A:THR:HG22 | 3        | 0.15          |
| (1,245) | 1:9:A:GLN:HE22  | 1:12:A:THR:HG23 | 3        | 0.15          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG21 | 5        | 0.15          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG22 | 5        | 0.15          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG23 | 5        | 0.15          |
| (1,245) | 1:9:A:GLN:HE22  | 1:12:A:THR:HG21 | 5        | 0.15          |
| (1,245) | 1:9:A:GLN:HE22  | 1:12:A:THR:HG22 | 5        | 0.15          |
| (1,245) | 1:9:A:GLN:HE22  | 1:12:A:THR:HG23 | 5        | 0.15          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG21 | 9        | 0.15          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG22 | 9        | 0.15          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,245) | 1:9:A:GLN:HE21 | 1:12:A:THR:HG23 | 9        | 0.15          |
| (1,245) | 1:9:A:GLN:HE22 | 1:12:A:THR:HG21 | 9        | 0.15          |
| (1,245) | 1:9:A:GLN:HE22 | 1:12:A:THR:HG22 | 9        | 0.15          |
| (1,245) | 1:9:A:GLN:HE22 | 1:12:A:THR:HG23 | 9        | 0.15          |
| (1,245) | 1:9:A:GLN:HE21 | 1:12:A:THR:HG21 | 11       | 0.15          |
| (1,245) | 1:9:A:GLN:HE21 | 1:12:A:THR:HG22 | 11       | 0.15          |
| (1,245) | 1:9:A:GLN:HE21 | 1:12:A:THR:HG23 | 11       | 0.15          |
| (1,245) | 1:9:A:GLN:HE22 | 1:12:A:THR:HG21 | 11       | 0.15          |
| (1,245) | 1:9:A:GLN:HE22 | 1:12:A:THR:HG22 | 11       | 0.15          |
| (1,245) | 1:9:A:GLN:HE22 | 1:12:A:THR:HG23 | 11       | 0.15          |
| (1,245) | 1:9:A:GLN:HE21 | 1:12:A:THR:HG21 | 17       | 0.15          |
| (1,245) | 1:9:A:GLN:HE21 | 1:12:A:THR:HG22 | 17       | 0.15          |
| (1,245) | 1:9:A:GLN:HE21 | 1:12:A:THR:HG23 | 17       | 0.15          |
| (1,245) | 1:9:A:GLN:HE22 | 1:12:A:THR:HG21 | 17       | 0.15          |
| (1,245) | 1:9:A:GLN:HE22 | 1:12:A:THR:HG22 | 17       | 0.15          |
| (1,245) | 1:9:A:GLN:HE22 | 1:12:A:THR:HG23 | 17       | 0.15          |
| (1,232) | 1:9:A:GLN:HA   | 1:9:A:GLN:HG2   | 16       | 0.15          |
| (1,232) | 1:9:A:GLN:HA   | 1:9:A:GLN:HG3   | 16       | 0.15          |
| (1,229) | 1:9:A:GLN:HB2  | 1:9:A:GLN:HE21  | 20       | 0.15          |
| (1,229) | 1:9:A:GLN:HB2  | 1:9:A:GLN:HE22  | 20       | 0.15          |
| (1,229) | 1:9:A:GLN:HB3  | 1:9:A:GLN:HE21  | 20       | 0.15          |
| (1,229) | 1:9:A:GLN:HB3  | 1:9:A:GLN:HE22  | 20       | 0.15          |
| (1,204) | 1:8:A:LEU:HB2  | 1:46:A:PHE:HE1  | 19       | 0.15          |
| (1,204) | 1:8:A:LEU:HB2  | 1:46:A:PHE:HE2  | 19       | 0.15          |
| (1,204) | 1:8:A:LEU:HB3  | 1:46:A:PHE:HE1  | 19       | 0.15          |
| (1,204) | 1:8:A:LEU:HB3  | 1:46:A:PHE:HE2  | 19       | 0.15          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD11  | 18       | 0.15          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD12  | 18       | 0.15          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD13  | 18       | 0.15          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD21  | 18       | 0.15          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD22  | 18       | 0.15          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD23  | 18       | 0.15          |
| (1,127) | 1:6:A:THR:HB   | 1:9:A:GLN:HG2   | 4        | 0.15          |
| (1,127) | 1:6:A:THR:HB   | 1:9:A:GLN:HG3   | 4        | 0.15          |
| (1,127) | 1:6:A:THR:HB   | 1:9:A:GLN:HG2   | 10       | 0.15          |
| (1,127) | 1:6:A:THR:HB   | 1:9:A:GLN:HG3   | 10       | 0.15          |
| (1,127) | 1:6:A:THR:HB   | 1:9:A:GLN:HG2   | 19       | 0.15          |
| (1,127) | 1:6:A:THR:HB   | 1:9:A:GLN:HG3   | 19       | 0.15          |
| (1,124) | 1:6:A:THR:HA   | 1:9:A:GLN:HG2   | 1        | 0.15          |
| (1,124) | 1:6:A:THR:HA   | 1:9:A:GLN:HG3   | 1        | 0.15          |
| (1,124) | 1:6:A:THR:HA   | 1:9:A:GLN:HG2   | 15       | 0.15          |
| (1,124) | 1:6:A:THR:HA   | 1:9:A:GLN:HG3   | 15       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,124)  | 1:6:A:THR:HA    | 1:9:A:GLN:HG2   | 18       | 0.15          |
| (1,124)  | 1:6:A:THR:HA    | 1:9:A:GLN:HG3   | 18       | 0.15          |
| (1,93)   | 1:4:A:TYR:HA    | 1:82:A:TYR:HE1  | 14       | 0.15          |
| (1,93)   | 1:4:A:TYR:HA    | 1:82:A:TYR:HE2  | 14       | 0.15          |
| (1,76)   | 1:4:A:TYR:HD1   | 1:56:A:ASP:HA   | 12       | 0.15          |
| (1,76)   | 1:4:A:TYR:HD2   | 1:56:A:ASP:HA   | 12       | 0.15          |
| (1,20)   | 1:2:A:ALA:HA    | 1:5:A:GLY:H     | 7        | 0.15          |
| (1,20)   | 1:2:A:ALA:HA    | 1:5:A:GLY:H     | 13       | 0.15          |
| (1,10)   | 1:1:A:MET:HA    | 1:57:A:LYS:HD2  | 19       | 0.15          |
| (1,10)   | 1:1:A:MET:HA    | 1:57:A:LYS:HD3  | 19       | 0.15          |
| (1,1900) | 1:89:A:ILE:HG21 | 1:90:A:SER:HB2  | 16       | 0.14          |
| (1,1900) | 1:89:A:ILE:HG21 | 1:90:A:SER:HB3  | 16       | 0.14          |
| (1,1900) | 1:89:A:ILE:HG22 | 1:90:A:SER:HB2  | 16       | 0.14          |
| (1,1900) | 1:89:A:ILE:HG22 | 1:90:A:SER:HB3  | 16       | 0.14          |
| (1,1900) | 1:89:A:ILE:HG23 | 1:90:A:SER:HB2  | 16       | 0.14          |
| (1,1900) | 1:89:A:ILE:HG23 | 1:90:A:SER:HB3  | 16       | 0.14          |
| (1,1888) | 1:89:A:ILE:HG21 | 1:89:A:ILE:H    | 1        | 0.14          |
| (1,1888) | 1:89:A:ILE:HG22 | 1:89:A:ILE:H    | 1        | 0.14          |
| (1,1888) | 1:89:A:ILE:HG23 | 1:89:A:ILE:H    | 1        | 0.14          |
| (1,1888) | 1:89:A:ILE:HG21 | 1:89:A:ILE:H    | 6        | 0.14          |
| (1,1888) | 1:89:A:ILE:HG22 | 1:89:A:ILE:H    | 6        | 0.14          |
| (1,1888) | 1:89:A:ILE:HG23 | 1:89:A:ILE:H    | 6        | 0.14          |
| (1,1888) | 1:89:A:ILE:HG21 | 1:89:A:ILE:H    | 7        | 0.14          |
| (1,1888) | 1:89:A:ILE:HG22 | 1:89:A:ILE:H    | 7        | 0.14          |
| (1,1888) | 1:89:A:ILE:HG23 | 1:89:A:ILE:H    | 7        | 0.14          |
| (1,1888) | 1:89:A:ILE:HG21 | 1:89:A:ILE:H    | 10       | 0.14          |
| (1,1888) | 1:89:A:ILE:HG22 | 1:89:A:ILE:H    | 10       | 0.14          |
| (1,1888) | 1:89:A:ILE:HG23 | 1:89:A:ILE:H    | 10       | 0.14          |
| (1,1888) | 1:89:A:ILE:HG21 | 1:89:A:ILE:H    | 11       | 0.14          |
| (1,1888) | 1:89:A:ILE:HG22 | 1:89:A:ILE:H    | 11       | 0.14          |
| (1,1888) | 1:89:A:ILE:HG23 | 1:89:A:ILE:H    | 11       | 0.14          |
| (1,1888) | 1:89:A:ILE:HG21 | 1:89:A:ILE:H    | 15       | 0.14          |
| (1,1888) | 1:89:A:ILE:HG22 | 1:89:A:ILE:H    | 15       | 0.14          |
| (1,1888) | 1:89:A:ILE:HG23 | 1:89:A:ILE:H    | 15       | 0.14          |
| (1,1874) | 1:87:A:LEU:HB2  | 1:89:A:ILE:HG21 | 20       | 0.14          |
| (1,1874) | 1:87:A:LEU:HB2  | 1:89:A:ILE:HG22 | 20       | 0.14          |
| (1,1874) | 1:87:A:LEU:HB2  | 1:89:A:ILE:HG23 | 20       | 0.14          |
| (1,1874) | 1:87:A:LEU:HB3  | 1:89:A:ILE:HG21 | 20       | 0.14          |
| (1,1874) | 1:87:A:LEU:HB3  | 1:89:A:ILE:HG22 | 20       | 0.14          |
| (1,1874) | 1:87:A:LEU:HB3  | 1:89:A:ILE:HG23 | 20       | 0.14          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD11 | 16       | 0.14          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD12 | 16       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD13 | 16       | 0.14          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD21 | 16       | 0.14          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD22 | 16       | 0.14          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD23 | 16       | 0.14          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD2  | 4        | 0.14          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD3  | 4        | 0.14          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD2  | 4        | 0.14          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD3  | 4        | 0.14          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD2  | 4        | 0.14          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD3  | 4        | 0.14          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD11 | 10       | 0.14          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD12 | 10       | 0.14          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD13 | 10       | 0.14          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD21 | 10       | 0.14          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD22 | 10       | 0.14          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD23 | 10       | 0.14          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD11 | 10       | 0.14          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD12 | 10       | 0.14          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD13 | 10       | 0.14          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD21 | 10       | 0.14          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD22 | 10       | 0.14          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD23 | 10       | 0.14          |
| (1,1794) | 1:83:A:ARG:HG2  | 1:84:A:THR:H    | 15       | 0.14          |
| (1,1794) | 1:83:A:ARG:HG3  | 1:84:A:THR:H    | 15       | 0.14          |
| (1,1794) | 1:83:A:ARG:HG2  | 1:84:A:THR:H    | 17       | 0.14          |
| (1,1794) | 1:83:A:ARG:HG3  | 1:84:A:THR:H    | 17       | 0.14          |
| (1,1785) | 1:82:A:TYR:HD1  | 1:89:A:ILE:HD11 | 7        | 0.14          |
| (1,1785) | 1:82:A:TYR:HD1  | 1:89:A:ILE:HD12 | 7        | 0.14          |
| (1,1785) | 1:82:A:TYR:HD1  | 1:89:A:ILE:HD13 | 7        | 0.14          |
| (1,1785) | 1:82:A:TYR:HD2  | 1:89:A:ILE:HD11 | 7        | 0.14          |
| (1,1785) | 1:82:A:TYR:HD2  | 1:89:A:ILE:HD12 | 7        | 0.14          |
| (1,1785) | 1:82:A:TYR:HD2  | 1:89:A:ILE:HD13 | 7        | 0.14          |
| (1,1777) | 1:82:A:TYR:HD1  | 1:85:A:ARG:HG2  | 2        | 0.14          |
| (1,1777) | 1:82:A:TYR:HD1  | 1:85:A:ARG:HG3  | 2        | 0.14          |
| (1,1777) | 1:82:A:TYR:HD2  | 1:85:A:ARG:HG2  | 2        | 0.14          |
| (1,1777) | 1:82:A:TYR:HD2  | 1:85:A:ARG:HG3  | 2        | 0.14          |
| (1,1777) | 1:82:A:TYR:HD1  | 1:85:A:ARG:HG2  | 12       | 0.14          |
| (1,1777) | 1:82:A:TYR:HD1  | 1:85:A:ARG:HG3  | 12       | 0.14          |
| (1,1777) | 1:82:A:TYR:HD2  | 1:85:A:ARG:HG2  | 12       | 0.14          |
| (1,1777) | 1:82:A:TYR:HD2  | 1:85:A:ARG:HG3  | 12       | 0.14          |
| (1,1762) | 1:82:A:TYR:HE1  | 1:82:A:TYR:H    | 2        | 0.14          |
| (1,1762) | 1:82:A:TYR:HE2  | 1:82:A:TYR:H    | 2        | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1735) | 1:80:A:VAL:HG11 | 1:81:A:ASP:HA   | 6        | 0.14          |
| (1,1735) | 1:80:A:VAL:HG12 | 1:81:A:ASP:HA   | 6        | 0.14          |
| (1,1735) | 1:80:A:VAL:HG13 | 1:81:A:ASP:HA   | 6        | 0.14          |
| (1,1735) | 1:80:A:VAL:HG21 | 1:81:A:ASP:HA   | 6        | 0.14          |
| (1,1735) | 1:80:A:VAL:HG22 | 1:81:A:ASP:HA   | 6        | 0.14          |
| (1,1735) | 1:80:A:VAL:HG23 | 1:81:A:ASP:HA   | 6        | 0.14          |
| (1,1680) | 1:77:A:THR:HG21 | 1:78:A:MET:HG2  | 15       | 0.14          |
| (1,1680) | 1:77:A:THR:HG21 | 1:78:A:MET:HG3  | 15       | 0.14          |
| (1,1680) | 1:77:A:THR:HG22 | 1:78:A:MET:HG2  | 15       | 0.14          |
| (1,1680) | 1:77:A:THR:HG22 | 1:78:A:MET:HG3  | 15       | 0.14          |
| (1,1680) | 1:77:A:THR:HG23 | 1:78:A:MET:HG2  | 15       | 0.14          |
| (1,1680) | 1:77:A:THR:HG23 | 1:78:A:MET:HG3  | 15       | 0.14          |
| (1,1669) | 1:76:A:LEU:HD11 | 1:80:A:VAL:HB   | 2        | 0.14          |
| (1,1669) | 1:76:A:LEU:HD12 | 1:80:A:VAL:HB   | 2        | 0.14          |
| (1,1669) | 1:76:A:LEU:HD13 | 1:80:A:VAL:HB   | 2        | 0.14          |
| (1,1669) | 1:76:A:LEU:HD21 | 1:80:A:VAL:HB   | 2        | 0.14          |
| (1,1669) | 1:76:A:LEU:HD22 | 1:80:A:VAL:HB   | 2        | 0.14          |
| (1,1669) | 1:76:A:LEU:HD23 | 1:80:A:VAL:HB   | 2        | 0.14          |
| (1,1669) | 1:76:A:LEU:HD11 | 1:80:A:VAL:HB   | 9        | 0.14          |
| (1,1669) | 1:76:A:LEU:HD12 | 1:80:A:VAL:HB   | 9        | 0.14          |
| (1,1669) | 1:76:A:LEU:HD13 | 1:80:A:VAL:HB   | 9        | 0.14          |
| (1,1669) | 1:76:A:LEU:HD21 | 1:80:A:VAL:HB   | 9        | 0.14          |
| (1,1669) | 1:76:A:LEU:HD22 | 1:80:A:VAL:HB   | 9        | 0.14          |
| (1,1669) | 1:76:A:LEU:HD23 | 1:80:A:VAL:HB   | 9        | 0.14          |
| (1,1609) | 1:73:A:PRO:HA   | 1:73:A:PRO:HG2  | 12       | 0.14          |
| (1,1609) | 1:73:A:PRO:HA   | 1:73:A:PRO:HG3  | 12       | 0.14          |
| (1,1597) | 1:72:A:ARG:HG2  | 1:74:A:ASP:H    | 12       | 0.14          |
| (1,1597) | 1:72:A:ARG:HG3  | 1:74:A:ASP:H    | 12       | 0.14          |
| (1,1576) | 1:71:A:ARG:HA   | 1:71:A:ARG:HG2  | 14       | 0.14          |
| (1,1576) | 1:71:A:ARG:HA   | 1:71:A:ARG:HG3  | 14       | 0.14          |
| (1,1525) | 1:68:A:GLU:HA   | 1:68:A:GLU:HG2  | 9        | 0.14          |
| (1,1525) | 1:68:A:GLU:HA   | 1:68:A:GLU:HG3  | 9        | 0.14          |
| (1,1439) | 1:65:A:HIS:HA   | 1:69:A:ILE:H    | 15       | 0.14          |
| (1,1428) | 1:65:A:HIS:HD2  | 1:66:A:ILE:HG12 | 4        | 0.14          |
| (1,1428) | 1:65:A:HIS:HD2  | 1:66:A:ILE:HG13 | 4        | 0.14          |
| (1,1428) | 1:65:A:HIS:HD2  | 1:66:A:ILE:HG12 | 10       | 0.14          |
| (1,1428) | 1:65:A:HIS:HD2  | 1:66:A:ILE:HG13 | 10       | 0.14          |
| (1,1355) | 1:63:A:ILE:HB   | 1:63:A:ILE:H    | 12       | 0.14          |
| (1,1355) | 1:63:A:ILE:HB   | 1:63:A:ILE:H    | 13       | 0.14          |
| (1,1355) | 1:63:A:ILE:HB   | 1:63:A:ILE:H    | 14       | 0.14          |
| (1,1355) | 1:63:A:ILE:HB   | 1:63:A:ILE:H    | 15       | 0.14          |
| (1,1355) | 1:63:A:ILE:HB   | 1:63:A:ILE:H    | 18       | 0.14          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG12 | 18       | 0.14          |
| (1,1351) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HG13 | 18       | 0.14          |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG12 | 18       | 0.14          |
| (1,1351) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HG13 | 18       | 0.14          |
| (1,1349) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HD11 | 9        | 0.14          |
| (1,1349) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HD12 | 9        | 0.14          |
| (1,1349) | 1:62:A:TYR:HE1 | 1:66:A:ILE:HD13 | 9        | 0.14          |
| (1,1349) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HD11 | 9        | 0.14          |
| (1,1349) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HD12 | 9        | 0.14          |
| (1,1349) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HD13 | 9        | 0.14          |
| (1,1336) | 1:62:A:TYR:HD1 | 1:63:A:ILE:HG21 | 18       | 0.14          |
| (1,1336) | 1:62:A:TYR:HD1 | 1:63:A:ILE:HG22 | 18       | 0.14          |
| (1,1336) | 1:62:A:TYR:HD1 | 1:63:A:ILE:HG23 | 18       | 0.14          |
| (1,1336) | 1:62:A:TYR:HD2 | 1:63:A:ILE:HG21 | 18       | 0.14          |
| (1,1336) | 1:62:A:TYR:HD2 | 1:63:A:ILE:HG22 | 18       | 0.14          |
| (1,1336) | 1:62:A:TYR:HD2 | 1:63:A:ILE:HG23 | 18       | 0.14          |
| (1,1324) | 1:61:A:SER:H   | 1:65:A:HIS:H    | 20       | 0.14          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG21 | 9        | 0.14          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG22 | 9        | 0.14          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG23 | 9        | 0.14          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG21 | 15       | 0.14          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG22 | 15       | 0.14          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG23 | 15       | 0.14          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD11 | 19       | 0.14          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD12 | 19       | 0.14          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD13 | 19       | 0.14          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD21 | 19       | 0.14          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD22 | 19       | 0.14          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD23 | 19       | 0.14          |
| (1,1277) | 1:58:A:ASP:H   | 1:60:A:LEU:H    | 4        | 0.14          |
| (1,1273) | 1:58:A:ASP:HA  | 1:59:A:ASN:HD21 | 8        | 0.14          |
| (1,1273) | 1:58:A:ASP:HA  | 1:59:A:ASN:HD22 | 8        | 0.14          |
| (1,1273) | 1:58:A:ASP:HA  | 1:59:A:ASN:HD21 | 17       | 0.14          |
| (1,1273) | 1:58:A:ASP:HA  | 1:59:A:ASN:HD22 | 17       | 0.14          |
| (1,1273) | 1:58:A:ASP:HA  | 1:59:A:ASN:HD21 | 18       | 0.14          |
| (1,1273) | 1:58:A:ASP:HA  | 1:59:A:ASN:HD22 | 18       | 0.14          |
| (1,1267) | 1:57:A:LYS:HD2 | 1:59:A:ASN:H    | 4        | 0.14          |
| (1,1267) | 1:57:A:LYS:HD3 | 1:59:A:ASN:H    | 4        | 0.14          |
| (1,1267) | 1:57:A:LYS:HD2 | 1:59:A:ASN:H    | 15       | 0.14          |
| (1,1267) | 1:57:A:LYS:HD3 | 1:59:A:ASN:H    | 15       | 0.14          |
| (1,1267) | 1:57:A:LYS:HD2 | 1:59:A:ASN:H    | 18       | 0.14          |
| (1,1267) | 1:57:A:LYS:HD3 | 1:59:A:ASN:H    | 18       | 0.14          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD2 | 18       | 0.14          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD3 | 18       | 0.14          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG2 | 11       | 0.14          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG3 | 11       | 0.14          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG2 | 19       | 0.14          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG3 | 19       | 0.14          |
| (1,1254) | 1:57:A:LYS:HD2 | 1:57:A:LYS:H   | 5        | 0.14          |
| (1,1254) | 1:57:A:LYS:HD3 | 1:57:A:LYS:H   | 5        | 0.14          |
| (1,1233) | 1:55:A:LEU:HG  | 1:63:A:ILE:HB  | 1        | 0.14          |
| (1,1233) | 1:55:A:LEU:HG  | 1:63:A:ILE:HB  | 16       | 0.14          |
| (1,1223) | 1:55:A:LEU:HG  | 1:56:A:ASP:HA  | 3        | 0.14          |
| (1,1223) | 1:55:A:LEU:HG  | 1:56:A:ASP:HA  | 16       | 0.14          |
| (1,1211) | 1:54:A:LYS:HB2 | 1:62:A:TYR:H   | 4        | 0.14          |
| (1,1211) | 1:54:A:LYS:HB3 | 1:62:A:TYR:H   | 4        | 0.14          |
| (1,1207) | 1:54:A:LYS:HG2 | 1:62:A:TYR:HE1 | 9        | 0.14          |
| (1,1207) | 1:54:A:LYS:HG2 | 1:62:A:TYR:HE2 | 9        | 0.14          |
| (1,1207) | 1:54:A:LYS:HG3 | 1:62:A:TYR:HE1 | 9        | 0.14          |
| (1,1207) | 1:54:A:LYS:HG3 | 1:62:A:TYR:HE2 | 9        | 0.14          |
| (1,1207) | 1:54:A:LYS:HG2 | 1:62:A:TYR:HE1 | 11       | 0.14          |
| (1,1207) | 1:54:A:LYS:HG2 | 1:62:A:TYR:HE2 | 11       | 0.14          |
| (1,1207) | 1:54:A:LYS:HG3 | 1:62:A:TYR:HE1 | 11       | 0.14          |
| (1,1207) | 1:54:A:LYS:HG3 | 1:62:A:TYR:HE2 | 11       | 0.14          |
| (1,1206) | 1:54:A:LYS:HB2 | 1:62:A:TYR:HE1 | 1        | 0.14          |
| (1,1206) | 1:54:A:LYS:HB2 | 1:62:A:TYR:HE2 | 1        | 0.14          |
| (1,1206) | 1:54:A:LYS:HB3 | 1:62:A:TYR:HE1 | 1        | 0.14          |
| (1,1206) | 1:54:A:LYS:HB3 | 1:62:A:TYR:HE2 | 1        | 0.14          |
| (1,1193) | 1:53:A:ASN:H   | 1:55:A:LEU:H   | 7        | 0.14          |
| (1,1168) | 1:52:A:HIS:HD2 | 1:52:A:HIS:HB2 | 1        | 0.14          |
| (1,1168) | 1:52:A:HIS:HD2 | 1:52:A:HIS:HB3 | 1        | 0.14          |
| (1,1062) | 1:47:A:SER:HA  | 1:51:A:SER:H   | 3        | 0.14          |
| (1,1062) | 1:47:A:SER:HA  | 1:51:A:SER:H   | 12       | 0.14          |
| (1,1018) | 1:46:A:PHE:HD1 | 1:46:A:PHE:H   | 14       | 0.14          |
| (1,1018) | 1:46:A:PHE:HD2 | 1:46:A:PHE:H   | 14       | 0.14          |
| (1,997)  | 1:45:A:TRP:HA  | 1:50:A:GLU:H   | 11       | 0.14          |
| (1,997)  | 1:45:A:TRP:HA  | 1:50:A:GLU:H   | 12       | 0.14          |
| (1,997)  | 1:45:A:TRP:HA  | 1:50:A:GLU:H   | 14       | 0.14          |
| (1,982)  | 1:45:A:TRP:HE1 | 1:46:A:PHE:HA  | 1        | 0.14          |
| (1,982)  | 1:45:A:TRP:HE1 | 1:46:A:PHE:HA  | 6        | 0.14          |
| (1,982)  | 1:45:A:TRP:HE1 | 1:46:A:PHE:HA  | 10       | 0.14          |
| (1,982)  | 1:45:A:TRP:HE1 | 1:46:A:PHE:HA  | 11       | 0.14          |
| (1,982)  | 1:45:A:TRP:HE1 | 1:46:A:PHE:HA  | 15       | 0.14          |
| (1,926)  | 1:41:A:THR:HB  | 1:42:A:GLY:H   | 3        | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,926) | 1:41:A:THR:HB   | 1:42:A:GLY:H    | 5        | 0.14          |
| (1,926) | 1:41:A:THR:HB   | 1:42:A:GLY:H    | 10       | 0.14          |
| (1,926) | 1:41:A:THR:HB   | 1:42:A:GLY:H    | 18       | 0.14          |
| (1,894) | 1:39:A:ILE:HD11 | 1:45:A:TRP:HH2  | 4        | 0.14          |
| (1,894) | 1:39:A:ILE:HD12 | 1:45:A:TRP:HH2  | 4        | 0.14          |
| (1,894) | 1:39:A:ILE:HD13 | 1:45:A:TRP:HH2  | 4        | 0.14          |
| (1,855) | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD11 | 3        | 0.14          |
| (1,855) | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD12 | 3        | 0.14          |
| (1,855) | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD13 | 3        | 0.14          |
| (1,855) | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD11 | 3        | 0.14          |
| (1,855) | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD12 | 3        | 0.14          |
| (1,855) | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD13 | 3        | 0.14          |
| (1,855) | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD11 | 7        | 0.14          |
| (1,855) | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD12 | 7        | 0.14          |
| (1,855) | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD13 | 7        | 0.14          |
| (1,855) | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD11 | 7        | 0.14          |
| (1,855) | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD12 | 7        | 0.14          |
| (1,855) | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD13 | 7        | 0.14          |
| (1,855) | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD11 | 10       | 0.14          |
| (1,855) | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD12 | 10       | 0.14          |
| (1,855) | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD13 | 10       | 0.14          |
| (1,855) | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD11 | 10       | 0.14          |
| (1,855) | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD12 | 10       | 0.14          |
| (1,855) | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD13 | 10       | 0.14          |
| (1,843) | 1:37:A:GLU:HA   | 1:37:A:GLU:HG2  | 18       | 0.14          |
| (1,843) | 1:37:A:GLU:HA   | 1:37:A:GLU:HG3  | 18       | 0.14          |
| (1,783) | 1:32:A:PRO:HD2  | 1:35:A:LYS:HG2  | 6        | 0.14          |
| (1,783) | 1:32:A:PRO:HD2  | 1:35:A:LYS:HG3  | 6        | 0.14          |
| (1,783) | 1:32:A:PRO:HD3  | 1:35:A:LYS:HG2  | 6        | 0.14          |
| (1,783) | 1:32:A:PRO:HD3  | 1:35:A:LYS:HG3  | 6        | 0.14          |
| (1,772) | 1:31:A:ILE:HG21 | 1:49:A:LEU:HA   | 20       | 0.14          |
| (1,772) | 1:31:A:ILE:HG22 | 1:49:A:LEU:HA   | 20       | 0.14          |
| (1,772) | 1:31:A:ILE:HG23 | 1:49:A:LEU:HA   | 20       | 0.14          |
| (1,743) | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD2  | 7        | 0.14          |
| (1,743) | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD3  | 7        | 0.14          |
| (1,743) | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD2  | 7        | 0.14          |
| (1,743) | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD3  | 7        | 0.14          |
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD2  | 7        | 0.14          |
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD3  | 7        | 0.14          |
| (1,743) | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD2  | 10       | 0.14          |
| (1,743) | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD3  | 10       | 0.14          |
| (1,743) | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD2  | 10       | 0.14          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,743) | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD3 | 10       | 0.14          |
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD2 | 10       | 0.14          |
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD3 | 10       | 0.14          |
| (1,743) | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD2 | 16       | 0.14          |
| (1,743) | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD3 | 16       | 0.14          |
| (1,743) | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD2 | 16       | 0.14          |
| (1,743) | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD3 | 16       | 0.14          |
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD2 | 16       | 0.14          |
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD3 | 16       | 0.14          |
| (1,743) | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD2 | 17       | 0.14          |
| (1,743) | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD3 | 17       | 0.14          |
| (1,743) | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD2 | 17       | 0.14          |
| (1,743) | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD3 | 17       | 0.14          |
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD2 | 17       | 0.14          |
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD3 | 17       | 0.14          |
| (1,736) | 1:31:A:ILE:HB   | 1:32:A:PRO:HA  | 9        | 0.14          |
| (1,724) | 1:31:A:ILE:HD11 | 1:31:A:ILE:H   | 1        | 0.14          |
| (1,724) | 1:31:A:ILE:HD12 | 1:31:A:ILE:H   | 1        | 0.14          |
| (1,724) | 1:31:A:ILE:HD13 | 1:31:A:ILE:H   | 1        | 0.14          |
| (1,724) | 1:31:A:ILE:HD11 | 1:31:A:ILE:H   | 5        | 0.14          |
| (1,724) | 1:31:A:ILE:HD12 | 1:31:A:ILE:H   | 5        | 0.14          |
| (1,724) | 1:31:A:ILE:HD13 | 1:31:A:ILE:H   | 5        | 0.14          |
| (1,724) | 1:31:A:ILE:HD11 | 1:31:A:ILE:H   | 10       | 0.14          |
| (1,724) | 1:31:A:ILE:HD12 | 1:31:A:ILE:H   | 10       | 0.14          |
| (1,724) | 1:31:A:ILE:HD13 | 1:31:A:ILE:H   | 10       | 0.14          |
| (1,724) | 1:31:A:ILE:HD11 | 1:31:A:ILE:H   | 13       | 0.14          |
| (1,724) | 1:31:A:ILE:HD12 | 1:31:A:ILE:H   | 13       | 0.14          |
| (1,724) | 1:31:A:ILE:HD13 | 1:31:A:ILE:H   | 13       | 0.14          |
| (1,724) | 1:31:A:ILE:HD11 | 1:31:A:ILE:H   | 15       | 0.14          |
| (1,724) | 1:31:A:ILE:HD12 | 1:31:A:ILE:H   | 15       | 0.14          |
| (1,724) | 1:31:A:ILE:HD13 | 1:31:A:ILE:H   | 15       | 0.14          |
| (1,705) | 1:29:A:GLU:HA   | 1:29:A:GLU:HG2 | 16       | 0.14          |
| (1,705) | 1:29:A:GLU:HA   | 1:29:A:GLU:HG3 | 16       | 0.14          |
| (1,627) | 1:24:A:LYS:HG2  | 1:45:A:TRP:HD1 | 13       | 0.14          |
| (1,627) | 1:24:A:LYS:HG3  | 1:45:A:TRP:HD1 | 13       | 0.14          |
| (1,627) | 1:24:A:LYS:HG2  | 1:45:A:TRP:HD1 | 17       | 0.14          |
| (1,627) | 1:24:A:LYS:HG3  | 1:45:A:TRP:HD1 | 17       | 0.14          |
| (1,555) | 1:22:A:GLN:HA   | 1:23:A:LEU:H   | 4        | 0.14          |
| (1,555) | 1:22:A:GLN:HA   | 1:23:A:LEU:H   | 5        | 0.14          |
| (1,555) | 1:22:A:GLN:HA   | 1:23:A:LEU:H   | 10       | 0.14          |
| (1,534) | 1:20:A:LEU:HD11 | 1:67:A:PHE:HE1 | 5        | 0.14          |
| (1,534) | 1:20:A:LEU:HD11 | 1:67:A:PHE:HE2 | 5        | 0.14          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,534) | 1:20:A:LEU:HD12 | 1:67:A:PHE:HE1 | 5        | 0.14          |
| (1,534) | 1:20:A:LEU:HD12 | 1:67:A:PHE:HE2 | 5        | 0.14          |
| (1,534) | 1:20:A:LEU:HD13 | 1:67:A:PHE:HE1 | 5        | 0.14          |
| (1,534) | 1:20:A:LEU:HD13 | 1:67:A:PHE:HE2 | 5        | 0.14          |
| (1,534) | 1:20:A:LEU:HD21 | 1:67:A:PHE:HE1 | 5        | 0.14          |
| (1,534) | 1:20:A:LEU:HD21 | 1:67:A:PHE:HE2 | 5        | 0.14          |
| (1,534) | 1:20:A:LEU:HD22 | 1:67:A:PHE:HE1 | 5        | 0.14          |
| (1,534) | 1:20:A:LEU:HD22 | 1:67:A:PHE:HE2 | 5        | 0.14          |
| (1,534) | 1:20:A:LEU:HD23 | 1:67:A:PHE:HE1 | 5        | 0.14          |
| (1,534) | 1:20:A:LEU:HD23 | 1:67:A:PHE:HE2 | 5        | 0.14          |
| (1,534) | 1:20:A:LEU:HD11 | 1:67:A:PHE:HE1 | 11       | 0.14          |
| (1,534) | 1:20:A:LEU:HD11 | 1:67:A:PHE:HE2 | 11       | 0.14          |
| (1,534) | 1:20:A:LEU:HD12 | 1:67:A:PHE:HE1 | 11       | 0.14          |
| (1,534) | 1:20:A:LEU:HD12 | 1:67:A:PHE:HE2 | 11       | 0.14          |
| (1,534) | 1:20:A:LEU:HD13 | 1:67:A:PHE:HE1 | 11       | 0.14          |
| (1,534) | 1:20:A:LEU:HD13 | 1:67:A:PHE:HE2 | 11       | 0.14          |
| (1,534) | 1:20:A:LEU:HD21 | 1:67:A:PHE:HE1 | 11       | 0.14          |
| (1,534) | 1:20:A:LEU:HD21 | 1:67:A:PHE:HE2 | 11       | 0.14          |
| (1,534) | 1:20:A:LEU:HD22 | 1:67:A:PHE:HE1 | 11       | 0.14          |
| (1,534) | 1:20:A:LEU:HD22 | 1:67:A:PHE:HE2 | 11       | 0.14          |
| (1,534) | 1:20:A:LEU:HD23 | 1:67:A:PHE:HE1 | 11       | 0.14          |
| (1,534) | 1:20:A:LEU:HD23 | 1:67:A:PHE:HE2 | 11       | 0.14          |
| (1,534) | 1:20:A:LEU:HD11 | 1:67:A:PHE:HE1 | 13       | 0.14          |
| (1,534) | 1:20:A:LEU:HD11 | 1:67:A:PHE:HE2 | 13       | 0.14          |
| (1,534) | 1:20:A:LEU:HD12 | 1:67:A:PHE:HE1 | 13       | 0.14          |
| (1,534) | 1:20:A:LEU:HD12 | 1:67:A:PHE:HE2 | 13       | 0.14          |
| (1,534) | 1:20:A:LEU:HD13 | 1:67:A:PHE:HE1 | 13       | 0.14          |
| (1,534) | 1:20:A:LEU:HD13 | 1:67:A:PHE:HE2 | 13       | 0.14          |
| (1,534) | 1:20:A:LEU:HD21 | 1:67:A:PHE:HE1 | 13       | 0.14          |
| (1,534) | 1:20:A:LEU:HD21 | 1:67:A:PHE:HE2 | 13       | 0.14          |
| (1,534) | 1:20:A:LEU:HD22 | 1:67:A:PHE:HE1 | 13       | 0.14          |
| (1,534) | 1:20:A:LEU:HD22 | 1:67:A:PHE:HE2 | 13       | 0.14          |
| (1,534) | 1:20:A:LEU:HD23 | 1:67:A:PHE:HE1 | 13       | 0.14          |
| (1,534) | 1:20:A:LEU:HD23 | 1:67:A:PHE:HE2 | 13       | 0.14          |
| (1,512) | 1:20:A:LEU:HB2  | 1:24:A:LYS:HG2 | 7        | 0.14          |
| (1,512) | 1:20:A:LEU:HB2  | 1:24:A:LYS:HG3 | 7        | 0.14          |
| (1,512) | 1:20:A:LEU:HB3  | 1:24:A:LYS:HG2 | 7        | 0.14          |
| (1,512) | 1:20:A:LEU:HB3  | 1:24:A:LYS:HG3 | 7        | 0.14          |
| (1,476) | 1:19:A:ASP:H    | 1:20:A:LEU:H   | 4        | 0.14          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB2 | 5        | 0.14          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB3 | 5        | 0.14          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB2 | 5        | 0.14          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB3 | 5        | 0.14          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB2 | 5        | 0.14          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB3 | 5        | 0.14          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB2 | 20       | 0.14          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB3 | 20       | 0.14          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB2 | 20       | 0.14          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB3 | 20       | 0.14          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB2 | 20       | 0.14          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB3 | 20       | 0.14          |
| (1,425) | 1:16:A:THR:HG21 | 1:18:A:GLU:H   | 13       | 0.14          |
| (1,425) | 1:16:A:THR:HG22 | 1:18:A:GLU:H   | 13       | 0.14          |
| (1,425) | 1:16:A:THR:HG23 | 1:18:A:GLU:H   | 13       | 0.14          |
| (1,425) | 1:16:A:THR:HG21 | 1:18:A:GLU:H   | 16       | 0.14          |
| (1,425) | 1:16:A:THR:HG22 | 1:18:A:GLU:H   | 16       | 0.14          |
| (1,425) | 1:16:A:THR:HG23 | 1:18:A:GLU:H   | 16       | 0.14          |
| (1,420) | 1:16:A:THR:HG21 | 1:17:A:LEU:H   | 7        | 0.14          |
| (1,420) | 1:16:A:THR:HG22 | 1:17:A:LEU:H   | 7        | 0.14          |
| (1,420) | 1:16:A:THR:HG23 | 1:17:A:LEU:H   | 7        | 0.14          |
| (1,420) | 1:16:A:THR:HG21 | 1:17:A:LEU:H   | 11       | 0.14          |
| (1,420) | 1:16:A:THR:HG22 | 1:17:A:LEU:H   | 11       | 0.14          |
| (1,420) | 1:16:A:THR:HG23 | 1:17:A:LEU:H   | 11       | 0.14          |
| (1,420) | 1:16:A:THR:HG21 | 1:17:A:LEU:H   | 13       | 0.14          |
| (1,420) | 1:16:A:THR:HG22 | 1:17:A:LEU:H   | 13       | 0.14          |
| (1,420) | 1:16:A:THR:HG23 | 1:17:A:LEU:H   | 13       | 0.14          |
| (1,420) | 1:16:A:THR:HG21 | 1:17:A:LEU:H   | 19       | 0.14          |
| (1,420) | 1:16:A:THR:HG22 | 1:17:A:LEU:H   | 19       | 0.14          |
| (1,420) | 1:16:A:THR:HG23 | 1:17:A:LEU:H   | 19       | 0.14          |
| (1,418) | 1:16:A:THR:HB   | 1:16:A:THR:H   | 20       | 0.14          |
| (1,405) | 1:15:A:ILE:HD11 | 1:43:A:SER:H   | 5        | 0.14          |
| (1,405) | 1:15:A:ILE:HD12 | 1:43:A:SER:H   | 5        | 0.14          |
| (1,405) | 1:15:A:ILE:HD13 | 1:43:A:SER:H   | 5        | 0.14          |
| (1,405) | 1:15:A:ILE:HD11 | 1:43:A:SER:H   | 13       | 0.14          |
| (1,405) | 1:15:A:ILE:HD12 | 1:43:A:SER:H   | 13       | 0.14          |
| (1,405) | 1:15:A:ILE:HD13 | 1:43:A:SER:H   | 13       | 0.14          |
| (1,373) | 1:14:A:ASN:HB2  | 1:75:A:LEU:HG  | 17       | 0.14          |
| (1,373) | 1:14:A:ASN:HB3  | 1:75:A:LEU:HG  | 17       | 0.14          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD1 | 8        | 0.14          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD2 | 8        | 0.14          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD1 | 8        | 0.14          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD2 | 8        | 0.14          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD1 | 8        | 0.14          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD2 | 8        | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD1  | 11       | 0.14          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD2  | 11       | 0.14          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD1  | 11       | 0.14          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD2  | 11       | 0.14          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD1  | 11       | 0.14          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD2  | 11       | 0.14          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD1  | 12       | 0.14          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD2  | 12       | 0.14          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD1  | 12       | 0.14          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD2  | 12       | 0.14          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD1  | 12       | 0.14          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD2  | 12       | 0.14          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD1  | 14       | 0.14          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD2  | 14       | 0.14          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD1  | 14       | 0.14          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD2  | 14       | 0.14          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD1  | 14       | 0.14          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD2  | 14       | 0.14          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD1  | 20       | 0.14          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD2  | 20       | 0.14          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD1  | 20       | 0.14          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD2  | 20       | 0.14          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD1  | 20       | 0.14          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD2  | 20       | 0.14          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG21 | 7        | 0.14          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG22 | 7        | 0.14          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG23 | 7        | 0.14          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG21 | 7        | 0.14          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG22 | 7        | 0.14          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG23 | 7        | 0.14          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG21 | 14       | 0.14          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG22 | 14       | 0.14          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG23 | 14       | 0.14          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG21 | 14       | 0.14          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG22 | 14       | 0.14          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG23 | 14       | 0.14          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG21 | 19       | 0.14          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG22 | 19       | 0.14          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG23 | 19       | 0.14          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG21 | 19       | 0.14          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG22 | 19       | 0.14          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG23 | 19       | 0.14          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,263) | 1:10:A:ASP:H   | 1:14:A:ASN:H    | 19       | 0.14          |
| (1,245) | 1:9:A:GLN:HE21 | 1:12:A:THR:HG21 | 4        | 0.14          |
| (1,245) | 1:9:A:GLN:HE21 | 1:12:A:THR:HG22 | 4        | 0.14          |
| (1,245) | 1:9:A:GLN:HE21 | 1:12:A:THR:HG23 | 4        | 0.14          |
| (1,245) | 1:9:A:GLN:HE22 | 1:12:A:THR:HG21 | 4        | 0.14          |
| (1,245) | 1:9:A:GLN:HE22 | 1:12:A:THR:HG22 | 4        | 0.14          |
| (1,245) | 1:9:A:GLN:HE22 | 1:12:A:THR:HG23 | 4        | 0.14          |
| (1,232) | 1:9:A:GLN:HA   | 1:9:A:GLN:HG2   | 14       | 0.14          |
| (1,232) | 1:9:A:GLN:HA   | 1:9:A:GLN:HG3   | 14       | 0.14          |
| (1,204) | 1:8:A:LEU:HB2  | 1:46:A:PHE:HE1  | 4        | 0.14          |
| (1,204) | 1:8:A:LEU:HB2  | 1:46:A:PHE:HE2  | 4        | 0.14          |
| (1,204) | 1:8:A:LEU:HB3  | 1:46:A:PHE:HE1  | 4        | 0.14          |
| (1,204) | 1:8:A:LEU:HB3  | 1:46:A:PHE:HE2  | 4        | 0.14          |
| (1,204) | 1:8:A:LEU:HB2  | 1:46:A:PHE:HE1  | 8        | 0.14          |
| (1,204) | 1:8:A:LEU:HB2  | 1:46:A:PHE:HE2  | 8        | 0.14          |
| (1,204) | 1:8:A:LEU:HB3  | 1:46:A:PHE:HE1  | 8        | 0.14          |
| (1,204) | 1:8:A:LEU:HB3  | 1:46:A:PHE:HE2  | 8        | 0.14          |
| (1,204) | 1:8:A:LEU:HB2  | 1:46:A:PHE:HE1  | 14       | 0.14          |
| (1,204) | 1:8:A:LEU:HB2  | 1:46:A:PHE:HE2  | 14       | 0.14          |
| (1,204) | 1:8:A:LEU:HB3  | 1:46:A:PHE:HE1  | 14       | 0.14          |
| (1,204) | 1:8:A:LEU:HB3  | 1:46:A:PHE:HE2  | 14       | 0.14          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD11  | 1        | 0.14          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD12  | 1        | 0.14          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD13  | 1        | 0.14          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD21  | 1        | 0.14          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD22  | 1        | 0.14          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD23  | 1        | 0.14          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD11  | 15       | 0.14          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD12  | 15       | 0.14          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD13  | 15       | 0.14          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD21  | 15       | 0.14          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD22  | 15       | 0.14          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD23  | 15       | 0.14          |
| (1,127) | 1:6:A:THR:HB   | 1:9:A:GLN:HG2   | 6        | 0.14          |
| (1,127) | 1:6:A:THR:HB   | 1:9:A:GLN:HG3   | 6        | 0.14          |
| (1,127) | 1:6:A:THR:HB   | 1:9:A:GLN:HG2   | 12       | 0.14          |
| (1,127) | 1:6:A:THR:HB   | 1:9:A:GLN:HG3   | 12       | 0.14          |
| (1,124) | 1:6:A:THR:HA   | 1:9:A:GLN:HG2   | 5        | 0.14          |
| (1,124) | 1:6:A:THR:HA   | 1:9:A:GLN:HG3   | 5        | 0.14          |
| (1,124) | 1:6:A:THR:HA   | 1:9:A:GLN:HG2   | 6        | 0.14          |
| (1,124) | 1:6:A:THR:HA   | 1:9:A:GLN:HG3   | 6        | 0.14          |
| (1,124) | 1:6:A:THR:HA   | 1:9:A:GLN:HG2   | 11       | 0.14          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,124) | 1:6:A:THR:HA  | 1:9:A:GLN:HG3  | 11       | 0.14          |
| (1,124) | 1:6:A:THR:HA  | 1:9:A:GLN:HG2  | 13       | 0.14          |
| (1,124) | 1:6:A:THR:HA  | 1:9:A:GLN:HG3  | 13       | 0.14          |
| (1,124) | 1:6:A:THR:HA  | 1:9:A:GLN:HG2  | 19       | 0.14          |
| (1,124) | 1:6:A:THR:HA  | 1:9:A:GLN:HG3  | 19       | 0.14          |
| (1,80)  | 1:4:A:TYR:HD1 | 1:57:A:LYS:HB2 | 7        | 0.14          |
| (1,80)  | 1:4:A:TYR:HD1 | 1:57:A:LYS:HB3 | 7        | 0.14          |
| (1,80)  | 1:4:A:TYR:HD2 | 1:57:A:LYS:HB2 | 7        | 0.14          |
| (1,80)  | 1:4:A:TYR:HD2 | 1:57:A:LYS:HB3 | 7        | 0.14          |
| (1,80)  | 1:4:A:TYR:HD1 | 1:57:A:LYS:HB2 | 20       | 0.14          |
| (1,80)  | 1:4:A:TYR:HD1 | 1:57:A:LYS:HB3 | 20       | 0.14          |
| (1,80)  | 1:4:A:TYR:HD2 | 1:57:A:LYS:HB2 | 20       | 0.14          |
| (1,80)  | 1:4:A:TYR:HD2 | 1:57:A:LYS:HB3 | 20       | 0.14          |
| (1,67)  | 1:4:A:TYR:HB2 | 1:7:A:LEU:HD11 | 5        | 0.14          |
| (1,67)  | 1:4:A:TYR:HB2 | 1:7:A:LEU:HD12 | 5        | 0.14          |
| (1,67)  | 1:4:A:TYR:HB2 | 1:7:A:LEU:HD13 | 5        | 0.14          |
| (1,67)  | 1:4:A:TYR:HB2 | 1:7:A:LEU:HD21 | 5        | 0.14          |
| (1,67)  | 1:4:A:TYR:HB2 | 1:7:A:LEU:HD22 | 5        | 0.14          |
| (1,67)  | 1:4:A:TYR:HB2 | 1:7:A:LEU:HD23 | 5        | 0.14          |
| (1,67)  | 1:4:A:TYR:HB3 | 1:7:A:LEU:HD11 | 5        | 0.14          |
| (1,67)  | 1:4:A:TYR:HB3 | 1:7:A:LEU:HD12 | 5        | 0.14          |
| (1,67)  | 1:4:A:TYR:HB3 | 1:7:A:LEU:HD13 | 5        | 0.14          |
| (1,67)  | 1:4:A:TYR:HB3 | 1:7:A:LEU:HD21 | 5        | 0.14          |
| (1,67)  | 1:4:A:TYR:HB3 | 1:7:A:LEU:HD22 | 5        | 0.14          |
| (1,67)  | 1:4:A:TYR:HB3 | 1:7:A:LEU:HD23 | 5        | 0.14          |
| (1,67)  | 1:4:A:TYR:HB2 | 1:7:A:LEU:HD11 | 6        | 0.14          |
| (1,67)  | 1:4:A:TYR:HB2 | 1:7:A:LEU:HD12 | 6        | 0.14          |
| (1,67)  | 1:4:A:TYR:HB2 | 1:7:A:LEU:HD13 | 6        | 0.14          |
| (1,67)  | 1:4:A:TYR:HB2 | 1:7:A:LEU:HD21 | 6        | 0.14          |
| (1,67)  | 1:4:A:TYR:HB2 | 1:7:A:LEU:HD22 | 6        | 0.14          |
| (1,67)  | 1:4:A:TYR:HB2 | 1:7:A:LEU:HD23 | 6        | 0.14          |
| (1,67)  | 1:4:A:TYR:HB3 | 1:7:A:LEU:HD11 | 6        | 0.14          |
| (1,67)  | 1:4:A:TYR:HB3 | 1:7:A:LEU:HD12 | 6        | 0.14          |
| (1,67)  | 1:4:A:TYR:HB3 | 1:7:A:LEU:HD13 | 6        | 0.14          |
| (1,67)  | 1:4:A:TYR:HB3 | 1:7:A:LEU:HD21 | 6        | 0.14          |
| (1,67)  | 1:4:A:TYR:HB3 | 1:7:A:LEU:HD22 | 6        | 0.14          |
| (1,67)  | 1:4:A:TYR:HB3 | 1:7:A:LEU:HD23 | 6        | 0.14          |
| (1,67)  | 1:4:A:TYR:HB2 | 1:7:A:LEU:HD11 | 11       | 0.14          |
| (1,67)  | 1:4:A:TYR:HB2 | 1:7:A:LEU:HD12 | 11       | 0.14          |
| (1,67)  | 1:4:A:TYR:HB2 | 1:7:A:LEU:HD13 | 11       | 0.14          |
| (1,67)  | 1:4:A:TYR:HB2 | 1:7:A:LEU:HD21 | 11       | 0.14          |
| (1,67)  | 1:4:A:TYR:HB2 | 1:7:A:LEU:HD22 | 11       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD23  | 11       | 0.14          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD11  | 11       | 0.14          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD12  | 11       | 0.14          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD13  | 11       | 0.14          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD21  | 11       | 0.14          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD22  | 11       | 0.14          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD23  | 11       | 0.14          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD11  | 20       | 0.14          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD12  | 20       | 0.14          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD13  | 20       | 0.14          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD21  | 20       | 0.14          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD22  | 20       | 0.14          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD23  | 20       | 0.14          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD11  | 20       | 0.14          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD12  | 20       | 0.14          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD13  | 20       | 0.14          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD21  | 20       | 0.14          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD22  | 20       | 0.14          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD23  | 20       | 0.14          |
| (1,38)   | 1:3:A:GLU:HG2   | 1:86:A:VAL:HG11 | 12       | 0.14          |
| (1,38)   | 1:3:A:GLU:HG2   | 1:86:A:VAL:HG12 | 12       | 0.14          |
| (1,38)   | 1:3:A:GLU:HG2   | 1:86:A:VAL:HG13 | 12       | 0.14          |
| (1,38)   | 1:3:A:GLU:HG2   | 1:86:A:VAL:HG21 | 12       | 0.14          |
| (1,38)   | 1:3:A:GLU:HG2   | 1:86:A:VAL:HG22 | 12       | 0.14          |
| (1,38)   | 1:3:A:GLU:HG2   | 1:86:A:VAL:HG23 | 12       | 0.14          |
| (1,38)   | 1:3:A:GLU:HG3   | 1:86:A:VAL:HG11 | 12       | 0.14          |
| (1,38)   | 1:3:A:GLU:HG3   | 1:86:A:VAL:HG12 | 12       | 0.14          |
| (1,38)   | 1:3:A:GLU:HG3   | 1:86:A:VAL:HG13 | 12       | 0.14          |
| (1,38)   | 1:3:A:GLU:HG3   | 1:86:A:VAL:HG21 | 12       | 0.14          |
| (1,38)   | 1:3:A:GLU:HG3   | 1:86:A:VAL:HG22 | 12       | 0.14          |
| (1,38)   | 1:3:A:GLU:HG3   | 1:86:A:VAL:HG23 | 12       | 0.14          |
| (1,25)   | 1:3:A:GLU:HG2   | 1:3:A:GLU:HA    | 5        | 0.14          |
| (1,25)   | 1:3:A:GLU:HG3   | 1:3:A:GLU:HA    | 5        | 0.14          |
| (1,25)   | 1:3:A:GLU:HG2   | 1:3:A:GLU:HA    | 13       | 0.14          |
| (1,25)   | 1:3:A:GLU:HG3   | 1:3:A:GLU:HA    | 13       | 0.14          |
| (1,20)   | 1:2:A:ALA:HA    | 1:5:A:GLY:H     | 2        | 0.14          |
| (1,20)   | 1:2:A:ALA:HA    | 1:5:A:GLY:H     | 3        | 0.14          |
| (1,20)   | 1:2:A:ALA:HA    | 1:5:A:GLY:H     | 19       | 0.14          |
| (1,6)    | 1:1:A:MET:HA    | 1:3:A:GLU:H     | 2        | 0.14          |
| (1,6)    | 1:1:A:MET:HA    | 1:3:A:GLU:H     | 5        | 0.14          |
| (1,1888) | 1:89:A:ILE:HG21 | 1:89:A:ILE:H    | 9        | 0.13          |
| (1,1888) | 1:89:A:ILE:HG22 | 1:89:A:ILE:H    | 9        | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1888) | 1:89:A:ILE:HG23 | 1:89:A:ILE:H    | 9        | 0.13          |
| (1,1888) | 1:89:A:ILE:HG21 | 1:89:A:ILE:H    | 17       | 0.13          |
| (1,1888) | 1:89:A:ILE:HG22 | 1:89:A:ILE:H    | 17       | 0.13          |
| (1,1888) | 1:89:A:ILE:HG23 | 1:89:A:ILE:H    | 17       | 0.13          |
| (1,1888) | 1:89:A:ILE:HG21 | 1:89:A:ILE:H    | 20       | 0.13          |
| (1,1888) | 1:89:A:ILE:HG22 | 1:89:A:ILE:H    | 20       | 0.13          |
| (1,1888) | 1:89:A:ILE:HG23 | 1:89:A:ILE:H    | 20       | 0.13          |
| (1,1838) | 1:85:A:ARG:H    | 1:86:A:VAL:HB   | 12       | 0.13          |
| (1,1834) | 1:85:A:ARG:HD2  | 1:86:A:VAL:HA   | 11       | 0.13          |
| (1,1834) | 1:85:A:ARG:HD3  | 1:86:A:VAL:HA   | 11       | 0.13          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD11 | 3        | 0.13          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD12 | 3        | 0.13          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD13 | 3        | 0.13          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD21 | 3        | 0.13          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD22 | 3        | 0.13          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD23 | 3        | 0.13          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD11 | 9        | 0.13          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD12 | 9        | 0.13          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD13 | 9        | 0.13          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD21 | 9        | 0.13          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD22 | 9        | 0.13          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD23 | 9        | 0.13          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD11 | 11       | 0.13          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD12 | 11       | 0.13          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD13 | 11       | 0.13          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD21 | 11       | 0.13          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD22 | 11       | 0.13          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD23 | 11       | 0.13          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD11 | 12       | 0.13          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD12 | 12       | 0.13          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD13 | 12       | 0.13          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD21 | 12       | 0.13          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD22 | 12       | 0.13          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD23 | 12       | 0.13          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD2  | 15       | 0.13          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD3  | 15       | 0.13          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD2  | 15       | 0.13          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD3  | 15       | 0.13          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD2  | 15       | 0.13          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD3  | 15       | 0.13          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD2  | 19       | 0.13          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD3  | 19       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD2  | 19       | 0.13          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD3  | 19       | 0.13          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD2  | 19       | 0.13          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD3  | 19       | 0.13          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD11 | 3        | 0.13          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD12 | 3        | 0.13          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD13 | 3        | 0.13          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD21 | 3        | 0.13          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD22 | 3        | 0.13          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD23 | 3        | 0.13          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD11 | 3        | 0.13          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD12 | 3        | 0.13          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD13 | 3        | 0.13          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD21 | 3        | 0.13          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD22 | 3        | 0.13          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD23 | 3        | 0.13          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD11 | 12       | 0.13          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD12 | 12       | 0.13          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD13 | 12       | 0.13          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD21 | 12       | 0.13          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD22 | 12       | 0.13          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD23 | 12       | 0.13          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD11 | 12       | 0.13          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD12 | 12       | 0.13          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD13 | 12       | 0.13          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD21 | 12       | 0.13          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD22 | 12       | 0.13          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD23 | 12       | 0.13          |
| (1,1794) | 1:83:A:ARG:HG2  | 1:84:A:THR:H    | 1        | 0.13          |
| (1,1794) | 1:83:A:ARG:HG3  | 1:84:A:THR:H    | 1        | 0.13          |
| (1,1794) | 1:83:A:ARG:HG2  | 1:84:A:THR:H    | 8        | 0.13          |
| (1,1794) | 1:83:A:ARG:HG3  | 1:84:A:THR:H    | 8        | 0.13          |
| (1,1794) | 1:83:A:ARG:HG2  | 1:84:A:THR:H    | 16       | 0.13          |
| (1,1794) | 1:83:A:ARG:HG3  | 1:84:A:THR:H    | 16       | 0.13          |
| (1,1762) | 1:82:A:TYR:HE1  | 1:82:A:TYR:H    | 16       | 0.13          |
| (1,1762) | 1:82:A:TYR:HE2  | 1:82:A:TYR:H    | 16       | 0.13          |
| (1,1745) | 1:80:A:VAL:HA   | 1:83:A:ARG:HD2  | 8        | 0.13          |
| (1,1745) | 1:80:A:VAL:HA   | 1:83:A:ARG:HD3  | 8        | 0.13          |
| (1,1745) | 1:80:A:VAL:HA   | 1:83:A:ARG:HD2  | 15       | 0.13          |
| (1,1745) | 1:80:A:VAL:HA   | 1:83:A:ARG:HD3  | 15       | 0.13          |
| (1,1693) | 1:77:A:THR:HG21 | 1:81:A:ASP:HB2  | 10       | 0.13          |
| (1,1693) | 1:77:A:THR:HG21 | 1:81:A:ASP:HB3  | 10       | 0.13          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1693) | 1:77:A:THR:HG22 | 1:81:A:ASP:HB2 | 10       | 0.13          |
| (1,1693) | 1:77:A:THR:HG22 | 1:81:A:ASP:HB3 | 10       | 0.13          |
| (1,1693) | 1:77:A:THR:HG23 | 1:81:A:ASP:HB2 | 10       | 0.13          |
| (1,1693) | 1:77:A:THR:HG23 | 1:81:A:ASP:HB3 | 10       | 0.13          |
| (1,1609) | 1:73:A:PRO:HA   | 1:73:A:PRO:HG2 | 7        | 0.13          |
| (1,1609) | 1:73:A:PRO:HA   | 1:73:A:PRO:HG3 | 7        | 0.13          |
| (1,1609) | 1:73:A:PRO:HA   | 1:73:A:PRO:HG2 | 8        | 0.13          |
| (1,1609) | 1:73:A:PRO:HA   | 1:73:A:PRO:HG3 | 8        | 0.13          |
| (1,1609) | 1:73:A:PRO:HA   | 1:73:A:PRO:HG2 | 13       | 0.13          |
| (1,1609) | 1:73:A:PRO:HA   | 1:73:A:PRO:HG3 | 13       | 0.13          |
| (1,1609) | 1:73:A:PRO:HA   | 1:73:A:PRO:HG2 | 16       | 0.13          |
| (1,1609) | 1:73:A:PRO:HA   | 1:73:A:PRO:HG3 | 16       | 0.13          |
| (1,1597) | 1:72:A:ARG:HG2  | 1:74:A:ASP:H   | 8        | 0.13          |
| (1,1597) | 1:72:A:ARG:HG3  | 1:74:A:ASP:H   | 8        | 0.13          |
| (1,1576) | 1:71:A:ARG:HA   | 1:71:A:ARG:HG2 | 7        | 0.13          |
| (1,1576) | 1:71:A:ARG:HA   | 1:71:A:ARG:HG3 | 7        | 0.13          |
| (1,1576) | 1:71:A:ARG:HA   | 1:71:A:ARG:HG2 | 8        | 0.13          |
| (1,1576) | 1:71:A:ARG:HA   | 1:71:A:ARG:HG3 | 8        | 0.13          |
| (1,1538) | 1:68:A:GLU:HA   | 1:71:A:ARG:HD2 | 4        | 0.13          |
| (1,1538) | 1:68:A:GLU:HA   | 1:71:A:ARG:HD3 | 4        | 0.13          |
| (1,1538) | 1:68:A:GLU:HA   | 1:71:A:ARG:HD2 | 7        | 0.13          |
| (1,1538) | 1:68:A:GLU:HA   | 1:71:A:ARG:HD3 | 7        | 0.13          |
| (1,1525) | 1:68:A:GLU:HA   | 1:68:A:GLU:HG2 | 4        | 0.13          |
| (1,1525) | 1:68:A:GLU:HA   | 1:68:A:GLU:HG3 | 4        | 0.13          |
| (1,1516) | 1:67:A:PHE:H    | 1:76:A:LEU:HG  | 1        | 0.13          |
| (1,1516) | 1:67:A:PHE:H    | 1:76:A:LEU:HG  | 8        | 0.13          |
| (1,1516) | 1:67:A:PHE:H    | 1:76:A:LEU:HG  | 9        | 0.13          |
| (1,1516) | 1:67:A:PHE:H    | 1:76:A:LEU:HG  | 11       | 0.13          |
| (1,1516) | 1:67:A:PHE:H    | 1:76:A:LEU:HG  | 12       | 0.13          |
| (1,1516) | 1:67:A:PHE:H    | 1:76:A:LEU:HG  | 13       | 0.13          |
| (1,1516) | 1:67:A:PHE:H    | 1:76:A:LEU:HG  | 14       | 0.13          |
| (1,1516) | 1:67:A:PHE:H    | 1:76:A:LEU:HG  | 16       | 0.13          |
| (1,1465) | 1:66:A:ILE:HD11 | 1:69:A:ILE:HA  | 9        | 0.13          |
| (1,1465) | 1:66:A:ILE:HD12 | 1:69:A:ILE:HA  | 9        | 0.13          |
| (1,1465) | 1:66:A:ILE:HD13 | 1:69:A:ILE:HA  | 9        | 0.13          |
| (1,1465) | 1:66:A:ILE:HD11 | 1:69:A:ILE:HA  | 10       | 0.13          |
| (1,1465) | 1:66:A:ILE:HD12 | 1:69:A:ILE:HA  | 10       | 0.13          |
| (1,1465) | 1:66:A:ILE:HD13 | 1:69:A:ILE:HA  | 10       | 0.13          |
| (1,1439) | 1:65:A:HIS:HA   | 1:69:A:ILE:H   | 1        | 0.13          |
| (1,1439) | 1:65:A:HIS:HA   | 1:69:A:ILE:H   | 3        | 0.13          |
| (1,1439) | 1:65:A:HIS:HA   | 1:69:A:ILE:H   | 10       | 0.13          |
| (1,1439) | 1:65:A:HIS:HA   | 1:69:A:ILE:H   | 12       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1439) | 1:65:A:HIS:HA   | 1:69:A:ILE:H    | 16       | 0.13          |
| (1,1439) | 1:65:A:HIS:HA   | 1:69:A:ILE:H    | 18       | 0.13          |
| (1,1437) | 1:65:A:HIS:HA   | 1:68:A:GLU:H    | 7        | 0.13          |
| (1,1428) | 1:65:A:HIS:HD2  | 1:66:A:ILE:HG12 | 8        | 0.13          |
| (1,1428) | 1:65:A:HIS:HD2  | 1:66:A:ILE:HG13 | 8        | 0.13          |
| (1,1428) | 1:65:A:HIS:HD2  | 1:66:A:ILE:HG12 | 9        | 0.13          |
| (1,1428) | 1:65:A:HIS:HD2  | 1:66:A:ILE:HG13 | 9        | 0.13          |
| (1,1399) | 1:64:A:GLU:HA   | 1:67:A:PHE:H    | 13       | 0.13          |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG11 | 17       | 0.13          |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG12 | 17       | 0.13          |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG13 | 17       | 0.13          |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG21 | 17       | 0.13          |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG22 | 17       | 0.13          |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG23 | 17       | 0.13          |
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG11 | 17       | 0.13          |
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG12 | 17       | 0.13          |
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG13 | 17       | 0.13          |
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG21 | 17       | 0.13          |
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG22 | 17       | 0.13          |
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG23 | 17       | 0.13          |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG11 | 17       | 0.13          |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG12 | 17       | 0.13          |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG13 | 17       | 0.13          |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG21 | 17       | 0.13          |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG22 | 17       | 0.13          |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG23 | 17       | 0.13          |
| (1,1379) | 1:63:A:ILE:HD11 | 1:67:A:PHE:H    | 1        | 0.13          |
| (1,1379) | 1:63:A:ILE:HD12 | 1:67:A:PHE:H    | 1        | 0.13          |
| (1,1379) | 1:63:A:ILE:HD13 | 1:67:A:PHE:H    | 1        | 0.13          |
| (1,1355) | 1:63:A:ILE:HB   | 1:63:A:ILE:H    | 4        | 0.13          |
| (1,1355) | 1:63:A:ILE:HB   | 1:63:A:ILE:H    | 7        | 0.13          |
| (1,1355) | 1:63:A:ILE:HB   | 1:63:A:ILE:H    | 8        | 0.13          |
| (1,1355) | 1:63:A:ILE:HB   | 1:63:A:ILE:H    | 9        | 0.13          |
| (1,1349) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HD11 | 6        | 0.13          |
| (1,1349) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HD12 | 6        | 0.13          |
| (1,1349) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HD13 | 6        | 0.13          |
| (1,1349) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HD11 | 6        | 0.13          |
| (1,1349) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HD12 | 6        | 0.13          |
| (1,1349) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HD13 | 6        | 0.13          |
| (1,1349) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HD11 | 10       | 0.13          |
| (1,1349) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HD12 | 10       | 0.13          |
| (1,1349) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HD13 | 10       | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1349) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HD11 | 10       | 0.13          |
| (1,1349) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HD12 | 10       | 0.13          |
| (1,1349) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HD13 | 10       | 0.13          |
| (1,1324) | 1:61:A:SER:H   | 1:65:A:HIS:H    | 19       | 0.13          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG21 | 4        | 0.13          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG22 | 4        | 0.13          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG23 | 4        | 0.13          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG21 | 6        | 0.13          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG22 | 6        | 0.13          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG23 | 6        | 0.13          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD11 | 15       | 0.13          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD12 | 15       | 0.13          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD13 | 15       | 0.13          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD21 | 15       | 0.13          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD22 | 15       | 0.13          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD23 | 15       | 0.13          |
| (1,1267) | 1:57:A:LYS:HD2 | 1:59:A:ASN:H    | 1        | 0.13          |
| (1,1267) | 1:57:A:LYS:HD3 | 1:59:A:ASN:H    | 1        | 0.13          |
| (1,1267) | 1:57:A:LYS:HD2 | 1:59:A:ASN:H    | 11       | 0.13          |
| (1,1267) | 1:57:A:LYS:HD3 | 1:59:A:ASN:H    | 11       | 0.13          |
| (1,1264) | 1:57:A:LYS:HG2 | 1:58:A:ASP:HA   | 16       | 0.13          |
| (1,1264) | 1:57:A:LYS:HG3 | 1:58:A:ASP:HA   | 16       | 0.13          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD2  | 13       | 0.13          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD3  | 13       | 0.13          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD2  | 14       | 0.13          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD3  | 14       | 0.13          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD2  | 19       | 0.13          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD3  | 19       | 0.13          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG2  | 2        | 0.13          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG3  | 2        | 0.13          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG2  | 3        | 0.13          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG3  | 3        | 0.13          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG2  | 4        | 0.13          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG3  | 4        | 0.13          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG2  | 14       | 0.13          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG3  | 14       | 0.13          |
| (1,1246) | 1:56:A:ASP:H   | 1:59:A:ASN:H    | 12       | 0.13          |
| (1,1233) | 1:55:A:LEU:HG  | 1:63:A:ILE:HB   | 8        | 0.13          |
| (1,1233) | 1:55:A:LEU:HG  | 1:63:A:ILE:HB   | 19       | 0.13          |
| (1,1233) | 1:55:A:LEU:HG  | 1:63:A:ILE:HB   | 20       | 0.13          |
| (1,1223) | 1:55:A:LEU:HG  | 1:56:A:ASP:HA   | 4        | 0.13          |
| (1,1223) | 1:55:A:LEU:HG  | 1:56:A:ASP:HA   | 15       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1206) | 1:54:A:LYS:HB2  | 1:62:A:TYR:HE1  | 14       | 0.13          |
| (1,1206) | 1:54:A:LYS:HB2  | 1:62:A:TYR:HE2  | 14       | 0.13          |
| (1,1206) | 1:54:A:LYS:HB3  | 1:62:A:TYR:HE1  | 14       | 0.13          |
| (1,1206) | 1:54:A:LYS:HB3  | 1:62:A:TYR:HE2  | 14       | 0.13          |
| (1,1194) | 1:54:A:LYS:HD2  | 1:54:A:LYS:H    | 8        | 0.13          |
| (1,1194) | 1:54:A:LYS:HD3  | 1:54:A:LYS:H    | 8        | 0.13          |
| (1,1194) | 1:54:A:LYS:HD2  | 1:54:A:LYS:H    | 15       | 0.13          |
| (1,1194) | 1:54:A:LYS:HD3  | 1:54:A:LYS:H    | 15       | 0.13          |
| (1,1132) | 1:49:A:LEU:HD11 | 1:63:A:ILE:HB   | 4        | 0.13          |
| (1,1132) | 1:49:A:LEU:HD12 | 1:63:A:ILE:HB   | 4        | 0.13          |
| (1,1132) | 1:49:A:LEU:HD13 | 1:63:A:ILE:HB   | 4        | 0.13          |
| (1,1132) | 1:49:A:LEU:HD21 | 1:63:A:ILE:HB   | 4        | 0.13          |
| (1,1132) | 1:49:A:LEU:HD22 | 1:63:A:ILE:HB   | 4        | 0.13          |
| (1,1132) | 1:49:A:LEU:HD23 | 1:63:A:ILE:HB   | 4        | 0.13          |
| (1,1107) | 1:49:A:LEU:HB2  | 1:52:A:HIS:HB2  | 20       | 0.13          |
| (1,1107) | 1:49:A:LEU:HB2  | 1:52:A:HIS:HB3  | 20       | 0.13          |
| (1,1107) | 1:49:A:LEU:HB3  | 1:52:A:HIS:HB2  | 20       | 0.13          |
| (1,1107) | 1:49:A:LEU:HB3  | 1:52:A:HIS:HB3  | 20       | 0.13          |
| (1,1085) | 1:48:A:PHE:HD1  | 1:52:A:HIS:HE1  | 16       | 0.13          |
| (1,1085) | 1:48:A:PHE:HD2  | 1:52:A:HIS:HE1  | 16       | 0.13          |
| (1,1062) | 1:47:A:SER:HA   | 1:51:A:SER:H    | 4        | 0.13          |
| (1,1062) | 1:47:A:SER:HA   | 1:51:A:SER:H    | 14       | 0.13          |
| (1,1018) | 1:46:A:PHE:HD1  | 1:46:A:PHE:H    | 9        | 0.13          |
| (1,1018) | 1:46:A:PHE:HD2  | 1:46:A:PHE:H    | 9        | 0.13          |
| (1,1010) | 1:45:A:TRP:HE1  | 1:66:A:ILE:HG12 | 11       | 0.13          |
| (1,1010) | 1:45:A:TRP:HE1  | 1:66:A:ILE:HG13 | 11       | 0.13          |
| (1,997)  | 1:45:A:TRP:HA   | 1:50:A:GLU:H    | 6        | 0.13          |
| (1,997)  | 1:45:A:TRP:HA   | 1:50:A:GLU:H    | 9        | 0.13          |
| (1,997)  | 1:45:A:TRP:HA   | 1:50:A:GLU:H    | 19       | 0.13          |
| (1,982)  | 1:45:A:TRP:HE1  | 1:46:A:PHE:HA   | 2        | 0.13          |
| (1,982)  | 1:45:A:TRP:HE1  | 1:46:A:PHE:HA   | 8        | 0.13          |
| (1,926)  | 1:41:A:THR:HB   | 1:42:A:GLY:H    | 14       | 0.13          |
| (1,918)  | 1:40:A:THR:HA   | 1:41:A:THR:H    | 18       | 0.13          |
| (1,909)  | 1:39:A:ILE:HG12 | 1:48:A:PHE:H    | 10       | 0.13          |
| (1,909)  | 1:39:A:ILE:HG13 | 1:48:A:PHE:H    | 10       | 0.13          |
| (1,901)  | 1:39:A:ILE:HG12 | 1:45:A:TRP:HD1  | 11       | 0.13          |
| (1,901)  | 1:39:A:ILE:HG13 | 1:45:A:TRP:HD1  | 11       | 0.13          |
| (1,898)  | 1:39:A:ILE:HG21 | 1:45:A:TRP:HB2  | 16       | 0.13          |
| (1,898)  | 1:39:A:ILE:HG21 | 1:45:A:TRP:HB3  | 16       | 0.13          |
| (1,898)  | 1:39:A:ILE:HG22 | 1:45:A:TRP:HB2  | 16       | 0.13          |
| (1,898)  | 1:39:A:ILE:HG22 | 1:45:A:TRP:HB3  | 16       | 0.13          |
| (1,898)  | 1:39:A:ILE:HG23 | 1:45:A:TRP:HB2  | 16       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,898) | 1:39:A:ILE:HG23 | 1:45:A:TRP:HB3  | 16       | 0.13          |
| (1,893) | 1:39:A:ILE:HD11 | 1:45:A:TRP:HD1  | 8        | 0.13          |
| (1,893) | 1:39:A:ILE:HD12 | 1:45:A:TRP:HD1  | 8        | 0.13          |
| (1,893) | 1:39:A:ILE:HD13 | 1:45:A:TRP:HD1  | 8        | 0.13          |
| (1,893) | 1:39:A:ILE:HD11 | 1:45:A:TRP:HD1  | 15       | 0.13          |
| (1,893) | 1:39:A:ILE:HD12 | 1:45:A:TRP:HD1  | 15       | 0.13          |
| (1,893) | 1:39:A:ILE:HD13 | 1:45:A:TRP:HD1  | 15       | 0.13          |
| (1,876) | 1:39:A:ILE:HD11 | 1:40:A:THR:HG21 | 2        | 0.13          |
| (1,876) | 1:39:A:ILE:HD11 | 1:40:A:THR:HG22 | 2        | 0.13          |
| (1,876) | 1:39:A:ILE:HD11 | 1:40:A:THR:HG23 | 2        | 0.13          |
| (1,876) | 1:39:A:ILE:HD12 | 1:40:A:THR:HG21 | 2        | 0.13          |
| (1,876) | 1:39:A:ILE:HD12 | 1:40:A:THR:HG22 | 2        | 0.13          |
| (1,876) | 1:39:A:ILE:HD12 | 1:40:A:THR:HG23 | 2        | 0.13          |
| (1,876) | 1:39:A:ILE:HD13 | 1:40:A:THR:HG21 | 2        | 0.13          |
| (1,876) | 1:39:A:ILE:HD13 | 1:40:A:THR:HG22 | 2        | 0.13          |
| (1,876) | 1:39:A:ILE:HD13 | 1:40:A:THR:HG23 | 2        | 0.13          |
| (1,876) | 1:39:A:ILE:HD11 | 1:40:A:THR:HG21 | 16       | 0.13          |
| (1,876) | 1:39:A:ILE:HD11 | 1:40:A:THR:HG22 | 16       | 0.13          |
| (1,876) | 1:39:A:ILE:HD11 | 1:40:A:THR:HG23 | 16       | 0.13          |
| (1,876) | 1:39:A:ILE:HD12 | 1:40:A:THR:HG21 | 16       | 0.13          |
| (1,876) | 1:39:A:ILE:HD12 | 1:40:A:THR:HG22 | 16       | 0.13          |
| (1,876) | 1:39:A:ILE:HD12 | 1:40:A:THR:HG23 | 16       | 0.13          |
| (1,876) | 1:39:A:ILE:HD13 | 1:40:A:THR:HG21 | 16       | 0.13          |
| (1,876) | 1:39:A:ILE:HD13 | 1:40:A:THR:HG22 | 16       | 0.13          |
| (1,876) | 1:39:A:ILE:HD13 | 1:40:A:THR:HG23 | 16       | 0.13          |
| (1,855) | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD11 | 15       | 0.13          |
| (1,855) | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD12 | 15       | 0.13          |
| (1,855) | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD13 | 15       | 0.13          |
| (1,855) | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD11 | 15       | 0.13          |
| (1,855) | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD12 | 15       | 0.13          |
| (1,855) | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD13 | 15       | 0.13          |
| (1,844) | 1:37:A:GLU:H    | 1:38:A:GLU:H    | 5        | 0.13          |
| (1,843) | 1:37:A:GLU:HA   | 1:37:A:GLU:HG2  | 11       | 0.13          |
| (1,843) | 1:37:A:GLU:HA   | 1:37:A:GLU:HG3  | 11       | 0.13          |
| (1,802) | 1:35:A:LYS:HA   | 1:35:A:LYS:HD2  | 1        | 0.13          |
| (1,802) | 1:35:A:LYS:HA   | 1:35:A:LYS:HD3  | 1        | 0.13          |
| (1,802) | 1:35:A:LYS:HA   | 1:35:A:LYS:HD2  | 10       | 0.13          |
| (1,802) | 1:35:A:LYS:HA   | 1:35:A:LYS:HD3  | 10       | 0.13          |
| (1,792) | 1:34:A:GLU:HA   | 1:34:A:GLU:HG2  | 11       | 0.13          |
| (1,792) | 1:34:A:GLU:HA   | 1:34:A:GLU:HG3  | 11       | 0.13          |
| (1,792) | 1:34:A:GLU:HA   | 1:34:A:GLU:HG2  | 17       | 0.13          |
| (1,792) | 1:34:A:GLU:HA   | 1:34:A:GLU:HG3  | 17       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,783) | 1:32:A:PRO:HD2  | 1:35:A:LYS:HG2  | 7        | 0.13          |
| (1,783) | 1:32:A:PRO:HD2  | 1:35:A:LYS:HG3  | 7        | 0.13          |
| (1,783) | 1:32:A:PRO:HD3  | 1:35:A:LYS:HG2  | 7        | 0.13          |
| (1,783) | 1:32:A:PRO:HD3  | 1:35:A:LYS:HG3  | 7        | 0.13          |
| (1,772) | 1:31:A:ILE:HG21 | 1:49:A:LEU:HA   | 19       | 0.13          |
| (1,772) | 1:31:A:ILE:HG22 | 1:49:A:LEU:HA   | 19       | 0.13          |
| (1,772) | 1:31:A:ILE:HG23 | 1:49:A:LEU:HA   | 19       | 0.13          |
| (1,761) | 1:31:A:ILE:HD11 | 1:45:A:TRP:HD1  | 7        | 0.13          |
| (1,761) | 1:31:A:ILE:HD12 | 1:45:A:TRP:HD1  | 7        | 0.13          |
| (1,761) | 1:31:A:ILE:HD13 | 1:45:A:TRP:HD1  | 7        | 0.13          |
| (1,761) | 1:31:A:ILE:HD11 | 1:45:A:TRP:HD1  | 13       | 0.13          |
| (1,761) | 1:31:A:ILE:HD12 | 1:45:A:TRP:HD1  | 13       | 0.13          |
| (1,761) | 1:31:A:ILE:HD13 | 1:45:A:TRP:HD1  | 13       | 0.13          |
| (1,736) | 1:31:A:ILE:HB   | 1:32:A:PRO:HA   | 3        | 0.13          |
| (1,736) | 1:31:A:ILE:HB   | 1:32:A:PRO:HA   | 16       | 0.13          |
| (1,724) | 1:31:A:ILE:HD11 | 1:31:A:ILE:H    | 2        | 0.13          |
| (1,724) | 1:31:A:ILE:HD12 | 1:31:A:ILE:H    | 2        | 0.13          |
| (1,724) | 1:31:A:ILE:HD13 | 1:31:A:ILE:H    | 2        | 0.13          |
| (1,724) | 1:31:A:ILE:HD11 | 1:31:A:ILE:H    | 3        | 0.13          |
| (1,724) | 1:31:A:ILE:HD12 | 1:31:A:ILE:H    | 3        | 0.13          |
| (1,724) | 1:31:A:ILE:HD13 | 1:31:A:ILE:H    | 3        | 0.13          |
| (1,724) | 1:31:A:ILE:HD11 | 1:31:A:ILE:H    | 9        | 0.13          |
| (1,724) | 1:31:A:ILE:HD12 | 1:31:A:ILE:H    | 9        | 0.13          |
| (1,724) | 1:31:A:ILE:HD13 | 1:31:A:ILE:H    | 9        | 0.13          |
| (1,724) | 1:31:A:ILE:HD11 | 1:31:A:ILE:H    | 12       | 0.13          |
| (1,724) | 1:31:A:ILE:HD12 | 1:31:A:ILE:H    | 12       | 0.13          |
| (1,724) | 1:31:A:ILE:HD13 | 1:31:A:ILE:H    | 12       | 0.13          |
| (1,669) | 1:27:A:CYS:HB2  | 1:30:A:ASP:H    | 13       | 0.13          |
| (1,669) | 1:27:A:CYS:HB3  | 1:30:A:ASP:H    | 13       | 0.13          |
| (1,669) | 1:27:A:CYS:HB2  | 1:30:A:ASP:H    | 15       | 0.13          |
| (1,669) | 1:27:A:CYS:HB3  | 1:30:A:ASP:H    | 15       | 0.13          |
| (1,626) | 1:24:A:LYS:HA   | 1:45:A:TRP:HE1  | 10       | 0.13          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG21 | 3        | 0.13          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG22 | 3        | 0.13          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG23 | 3        | 0.13          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG21 | 5        | 0.13          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG22 | 5        | 0.13          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG23 | 5        | 0.13          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG21 | 8        | 0.13          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG22 | 8        | 0.13          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG23 | 8        | 0.13          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG21 | 13       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG22 | 13       | 0.13          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG23 | 13       | 0.13          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG21 | 19       | 0.13          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG22 | 19       | 0.13          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG23 | 19       | 0.13          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG21 | 7        | 0.13          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG22 | 7        | 0.13          |
| (1,570) | 1:22:A:GLN:H    | 1:66:A:ILE:HG23 | 7        | 0.13          |
| (1,565) | 1:22:A:GLN:HB2  | 1:25:A:SER:H    | 18       | 0.13          |
| (1,565) | 1:22:A:GLN:HB3  | 1:25:A:SER:H    | 18       | 0.13          |
| (1,557) | 1:22:A:GLN:HE21 | 1:23:A:LEU:HA   | 4        | 0.13          |
| (1,557) | 1:22:A:GLN:HE22 | 1:23:A:LEU:HA   | 4        | 0.13          |
| (1,555) | 1:22:A:GLN:HA   | 1:23:A:LEU:H    | 7        | 0.13          |
| (1,555) | 1:22:A:GLN:HA   | 1:23:A:LEU:H    | 13       | 0.13          |
| (1,555) | 1:22:A:GLN:HA   | 1:23:A:LEU:H    | 17       | 0.13          |
| (1,555) | 1:22:A:GLN:HA   | 1:23:A:LEU:H    | 19       | 0.13          |
| (1,534) | 1:20:A:LEU:HD11 | 1:67:A:PHE:HE1  | 1        | 0.13          |
| (1,534) | 1:20:A:LEU:HD11 | 1:67:A:PHE:HE2  | 1        | 0.13          |
| (1,534) | 1:20:A:LEU:HD12 | 1:67:A:PHE:HE1  | 1        | 0.13          |
| (1,534) | 1:20:A:LEU:HD12 | 1:67:A:PHE:HE2  | 1        | 0.13          |
| (1,534) | 1:20:A:LEU:HD13 | 1:67:A:PHE:HE1  | 1        | 0.13          |
| (1,534) | 1:20:A:LEU:HD13 | 1:67:A:PHE:HE2  | 1        | 0.13          |
| (1,534) | 1:20:A:LEU:HD21 | 1:67:A:PHE:HE1  | 1        | 0.13          |
| (1,534) | 1:20:A:LEU:HD21 | 1:67:A:PHE:HE2  | 1        | 0.13          |
| (1,534) | 1:20:A:LEU:HD22 | 1:67:A:PHE:HE1  | 1        | 0.13          |
| (1,534) | 1:20:A:LEU:HD22 | 1:67:A:PHE:HE2  | 1        | 0.13          |
| (1,534) | 1:20:A:LEU:HD23 | 1:67:A:PHE:HE1  | 1        | 0.13          |
| (1,534) | 1:20:A:LEU:HD23 | 1:67:A:PHE:HE2  | 1        | 0.13          |
| (1,534) | 1:20:A:LEU:HD11 | 1:67:A:PHE:HE1  | 6        | 0.13          |
| (1,534) | 1:20:A:LEU:HD11 | 1:67:A:PHE:HE2  | 6        | 0.13          |
| (1,534) | 1:20:A:LEU:HD12 | 1:67:A:PHE:HE1  | 6        | 0.13          |
| (1,534) | 1:20:A:LEU:HD12 | 1:67:A:PHE:HE2  | 6        | 0.13          |
| (1,534) | 1:20:A:LEU:HD13 | 1:67:A:PHE:HE1  | 6        | 0.13          |
| (1,534) | 1:20:A:LEU:HD13 | 1:67:A:PHE:HE2  | 6        | 0.13          |
| (1,534) | 1:20:A:LEU:HD21 | 1:67:A:PHE:HE1  | 6        | 0.13          |
| (1,534) | 1:20:A:LEU:HD21 | 1:67:A:PHE:HE2  | 6        | 0.13          |
| (1,534) | 1:20:A:LEU:HD22 | 1:67:A:PHE:HE1  | 6        | 0.13          |
| (1,534) | 1:20:A:LEU:HD22 | 1:67:A:PHE:HE2  | 6        | 0.13          |
| (1,534) | 1:20:A:LEU:HD23 | 1:67:A:PHE:HE1  | 6        | 0.13          |
| (1,534) | 1:20:A:LEU:HD23 | 1:67:A:PHE:HE2  | 6        | 0.13          |
| (1,534) | 1:20:A:LEU:HD11 | 1:67:A:PHE:HE1  | 9        | 0.13          |
| (1,534) | 1:20:A:LEU:HD11 | 1:67:A:PHE:HE2  | 9        | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,534) | 1:20:A:LEU:HD12 | 1:67:A:PHE:HE1  | 9        | 0.13          |
| (1,534) | 1:20:A:LEU:HD12 | 1:67:A:PHE:HE2  | 9        | 0.13          |
| (1,534) | 1:20:A:LEU:HD13 | 1:67:A:PHE:HE1  | 9        | 0.13          |
| (1,534) | 1:20:A:LEU:HD13 | 1:67:A:PHE:HE2  | 9        | 0.13          |
| (1,534) | 1:20:A:LEU:HD21 | 1:67:A:PHE:HE1  | 9        | 0.13          |
| (1,534) | 1:20:A:LEU:HD21 | 1:67:A:PHE:HE2  | 9        | 0.13          |
| (1,534) | 1:20:A:LEU:HD22 | 1:67:A:PHE:HE1  | 9        | 0.13          |
| (1,534) | 1:20:A:LEU:HD22 | 1:67:A:PHE:HE2  | 9        | 0.13          |
| (1,534) | 1:20:A:LEU:HD23 | 1:67:A:PHE:HE1  | 9        | 0.13          |
| (1,534) | 1:20:A:LEU:HD23 | 1:67:A:PHE:HE2  | 9        | 0.13          |
| (1,516) | 1:20:A:LEU:HD11 | 1:39:A:ILE:HD11 | 4        | 0.13          |
| (1,516) | 1:20:A:LEU:HD11 | 1:39:A:ILE:HD12 | 4        | 0.13          |
| (1,516) | 1:20:A:LEU:HD11 | 1:39:A:ILE:HD13 | 4        | 0.13          |
| (1,516) | 1:20:A:LEU:HD12 | 1:39:A:ILE:HD11 | 4        | 0.13          |
| (1,516) | 1:20:A:LEU:HD12 | 1:39:A:ILE:HD12 | 4        | 0.13          |
| (1,516) | 1:20:A:LEU:HD12 | 1:39:A:ILE:HD13 | 4        | 0.13          |
| (1,516) | 1:20:A:LEU:HD13 | 1:39:A:ILE:HD11 | 4        | 0.13          |
| (1,516) | 1:20:A:LEU:HD13 | 1:39:A:ILE:HD12 | 4        | 0.13          |
| (1,516) | 1:20:A:LEU:HD13 | 1:39:A:ILE:HD13 | 4        | 0.13          |
| (1,516) | 1:20:A:LEU:HD21 | 1:39:A:ILE:HD11 | 4        | 0.13          |
| (1,516) | 1:20:A:LEU:HD21 | 1:39:A:ILE:HD12 | 4        | 0.13          |
| (1,516) | 1:20:A:LEU:HD21 | 1:39:A:ILE:HD13 | 4        | 0.13          |
| (1,516) | 1:20:A:LEU:HD22 | 1:39:A:ILE:HD11 | 4        | 0.13          |
| (1,516) | 1:20:A:LEU:HD22 | 1:39:A:ILE:HD12 | 4        | 0.13          |
| (1,516) | 1:20:A:LEU:HD22 | 1:39:A:ILE:HD13 | 4        | 0.13          |
| (1,516) | 1:20:A:LEU:HD23 | 1:39:A:ILE:HD11 | 4        | 0.13          |
| (1,516) | 1:20:A:LEU:HD23 | 1:39:A:ILE:HD12 | 4        | 0.13          |
| (1,516) | 1:20:A:LEU:HD23 | 1:39:A:ILE:HD13 | 4        | 0.13          |
| (1,487) | 1:20:A:LEU:HG   | 1:20:A:LEU:H    | 2        | 0.13          |
| (1,476) | 1:19:A:ASP:H    | 1:20:A:LEU:H    | 3        | 0.13          |
| (1,476) | 1:19:A:ASP:H    | 1:20:A:LEU:H    | 13       | 0.13          |
| (1,469) | 1:18:A:GLU:HA   | 1:20:A:LEU:HB2  | 2        | 0.13          |
| (1,469) | 1:18:A:GLU:HA   | 1:20:A:LEU:HB3  | 2        | 0.13          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB2  | 7        | 0.13          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB3  | 7        | 0.13          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB2  | 7        | 0.13          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB3  | 7        | 0.13          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB2  | 7        | 0.13          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB3  | 7        | 0.13          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB2  | 8        | 0.13          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB3  | 8        | 0.13          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB2  | 8        | 0.13          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB3 | 8        | 0.13          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB2 | 8        | 0.13          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB3 | 8        | 0.13          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB2 | 11       | 0.13          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB3 | 11       | 0.13          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB2 | 11       | 0.13          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB3 | 11       | 0.13          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB2 | 11       | 0.13          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB3 | 11       | 0.13          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB2 | 15       | 0.13          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB3 | 15       | 0.13          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB2 | 15       | 0.13          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB3 | 15       | 0.13          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB2 | 15       | 0.13          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB3 | 15       | 0.13          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB2 | 16       | 0.13          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB3 | 16       | 0.13          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB2 | 16       | 0.13          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB3 | 16       | 0.13          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB2 | 16       | 0.13          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB3 | 16       | 0.13          |
| (1,425) | 1:16:A:THR:HG21 | 1:18:A:GLU:H   | 1        | 0.13          |
| (1,425) | 1:16:A:THR:HG22 | 1:18:A:GLU:H   | 1        | 0.13          |
| (1,425) | 1:16:A:THR:HG23 | 1:18:A:GLU:H   | 1        | 0.13          |
| (1,425) | 1:16:A:THR:HG21 | 1:18:A:GLU:H   | 4        | 0.13          |
| (1,425) | 1:16:A:THR:HG22 | 1:18:A:GLU:H   | 4        | 0.13          |
| (1,425) | 1:16:A:THR:HG23 | 1:18:A:GLU:H   | 4        | 0.13          |
| (1,425) | 1:16:A:THR:HG21 | 1:18:A:GLU:H   | 11       | 0.13          |
| (1,425) | 1:16:A:THR:HG22 | 1:18:A:GLU:H   | 11       | 0.13          |
| (1,425) | 1:16:A:THR:HG23 | 1:18:A:GLU:H   | 11       | 0.13          |
| (1,418) | 1:16:A:THR:HB   | 1:16:A:THR:H   | 10       | 0.13          |
| (1,418) | 1:16:A:THR:HB   | 1:16:A:THR:H   | 12       | 0.13          |
| (1,405) | 1:15:A:ILE:HD11 | 1:43:A:SER:H   | 9        | 0.13          |
| (1,405) | 1:15:A:ILE:HD12 | 1:43:A:SER:H   | 9        | 0.13          |
| (1,405) | 1:15:A:ILE:HD13 | 1:43:A:SER:H   | 9        | 0.13          |
| (1,405) | 1:15:A:ILE:HD11 | 1:43:A:SER:H   | 12       | 0.13          |
| (1,405) | 1:15:A:ILE:HD12 | 1:43:A:SER:H   | 12       | 0.13          |
| (1,405) | 1:15:A:ILE:HD13 | 1:43:A:SER:H   | 12       | 0.13          |
| (1,405) | 1:15:A:ILE:HD11 | 1:43:A:SER:H   | 17       | 0.13          |
| (1,405) | 1:15:A:ILE:HD12 | 1:43:A:SER:H   | 17       | 0.13          |
| (1,405) | 1:15:A:ILE:HD13 | 1:43:A:SER:H   | 17       | 0.13          |
| (1,387) | 1:15:A:ILE:HD11 | 1:19:A:ASP:H   | 12       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,387) | 1:15:A:ILE:HD12 | 1:19:A:ASP:H    | 12       | 0.13          |
| (1,387) | 1:15:A:ILE:HD13 | 1:19:A:ASP:H    | 12       | 0.13          |
| (1,357) | 1:13:A:ASN:H    | 1:75:A:LEU:HG   | 19       | 0.13          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD1  | 4        | 0.13          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD2  | 4        | 0.13          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD1  | 4        | 0.13          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD2  | 4        | 0.13          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD1  | 4        | 0.13          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD2  | 4        | 0.13          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD1  | 10       | 0.13          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD2  | 10       | 0.13          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD1  | 10       | 0.13          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD2  | 10       | 0.13          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD1  | 10       | 0.13          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD2  | 10       | 0.13          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD1  | 13       | 0.13          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD2  | 13       | 0.13          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD1  | 13       | 0.13          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD2  | 13       | 0.13          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD1  | 13       | 0.13          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD2  | 13       | 0.13          |
| (1,335) | 1:12:A:THR:HB   | 1:42:A:GLY:H    | 19       | 0.13          |
| (1,304) | 1:11:A:LEU:HD11 | 1:75:A:LEU:HG   | 12       | 0.13          |
| (1,304) | 1:11:A:LEU:HD12 | 1:75:A:LEU:HG   | 12       | 0.13          |
| (1,304) | 1:11:A:LEU:HD13 | 1:75:A:LEU:HG   | 12       | 0.13          |
| (1,304) | 1:11:A:LEU:HD21 | 1:75:A:LEU:HG   | 12       | 0.13          |
| (1,304) | 1:11:A:LEU:HD22 | 1:75:A:LEU:HG   | 12       | 0.13          |
| (1,304) | 1:11:A:LEU:HD23 | 1:75:A:LEU:HG   | 12       | 0.13          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD11 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD12 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD13 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD21 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD22 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD23 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD11 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD12 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD13 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD21 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD22 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD23 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD11 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD12 | 16       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD13 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD21 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD22 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD23 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD11 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD12 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD13 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD21 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD22 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD23 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD11 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD12 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD13 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD21 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD22 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD23 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD11 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD12 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD13 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD21 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD22 | 16       | 0.13          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD23 | 16       | 0.13          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG21 | 13       | 0.13          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG22 | 13       | 0.13          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG23 | 13       | 0.13          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG21 | 13       | 0.13          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG22 | 13       | 0.13          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG23 | 13       | 0.13          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG21 | 20       | 0.13          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG22 | 20       | 0.13          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG23 | 20       | 0.13          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG21 | 20       | 0.13          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG22 | 20       | 0.13          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG23 | 20       | 0.13          |
| (1,263) | 1:10:A:ASP:H    | 1:14:A:ASN:H    | 6        | 0.13          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG21 | 18       | 0.13          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG22 | 18       | 0.13          |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG23 | 18       | 0.13          |
| (1,245) | 1:9:A:GLN:HE22  | 1:12:A:THR:HG21 | 18       | 0.13          |
| (1,245) | 1:9:A:GLN:HE22  | 1:12:A:THR:HG22 | 18       | 0.13          |
| (1,245) | 1:9:A:GLN:HE22  | 1:12:A:THR:HG23 | 18       | 0.13          |
| (1,204) | 1:8:A:LEU:HB2   | 1:46:A:PHE:HE1  | 3        | 0.13          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,204) | 1:8:A:LEU:HB2 | 1:46:A:PHE:HE2 | 3        | 0.13          |
| (1,204) | 1:8:A:LEU:HB3 | 1:46:A:PHE:HE1 | 3        | 0.13          |
| (1,204) | 1:8:A:LEU:HB3 | 1:46:A:PHE:HE2 | 3        | 0.13          |
| (1,204) | 1:8:A:LEU:HB2 | 1:46:A:PHE:HE1 | 20       | 0.13          |
| (1,204) | 1:8:A:LEU:HB2 | 1:46:A:PHE:HE2 | 20       | 0.13          |
| (1,204) | 1:8:A:LEU:HB3 | 1:46:A:PHE:HE1 | 20       | 0.13          |
| (1,204) | 1:8:A:LEU:HB3 | 1:46:A:PHE:HE2 | 20       | 0.13          |
| (1,147) | 1:7:A:LEU:HG  | 1:8:A:LEU:HD11 | 16       | 0.13          |
| (1,147) | 1:7:A:LEU:HG  | 1:8:A:LEU:HD12 | 16       | 0.13          |
| (1,147) | 1:7:A:LEU:HG  | 1:8:A:LEU:HD13 | 16       | 0.13          |
| (1,147) | 1:7:A:LEU:HG  | 1:8:A:LEU:HD21 | 16       | 0.13          |
| (1,147) | 1:7:A:LEU:HG  | 1:8:A:LEU:HD22 | 16       | 0.13          |
| (1,147) | 1:7:A:LEU:HG  | 1:8:A:LEU:HD23 | 16       | 0.13          |
| (1,127) | 1:6:A:THR:HB  | 1:9:A:GLN:HG2  | 7        | 0.13          |
| (1,127) | 1:6:A:THR:HB  | 1:9:A:GLN:HG3  | 7        | 0.13          |
| (1,127) | 1:6:A:THR:HB  | 1:9:A:GLN:HG2  | 18       | 0.13          |
| (1,127) | 1:6:A:THR:HB  | 1:9:A:GLN:HG3  | 18       | 0.13          |
| (1,124) | 1:6:A:THR:HA  | 1:9:A:GLN:HG2  | 4        | 0.13          |
| (1,124) | 1:6:A:THR:HA  | 1:9:A:GLN:HG3  | 4        | 0.13          |
| (1,124) | 1:6:A:THR:HA  | 1:9:A:GLN:HG2  | 8        | 0.13          |
| (1,124) | 1:6:A:THR:HA  | 1:9:A:GLN:HG3  | 8        | 0.13          |
| (1,93)  | 1:4:A:TYR:HA  | 1:82:A:TYR:HE1 | 16       | 0.13          |
| (1,93)  | 1:4:A:TYR:HA  | 1:82:A:TYR:HE2 | 16       | 0.13          |
| (1,76)  | 1:4:A:TYR:HD1 | 1:56:A:ASP:HA  | 15       | 0.13          |
| (1,76)  | 1:4:A:TYR:HD2 | 1:56:A:ASP:HA  | 15       | 0.13          |
| (1,67)  | 1:4:A:TYR:HB2 | 1:7:A:LEU:HD11 | 7        | 0.13          |
| (1,67)  | 1:4:A:TYR:HB2 | 1:7:A:LEU:HD12 | 7        | 0.13          |
| (1,67)  | 1:4:A:TYR:HB2 | 1:7:A:LEU:HD13 | 7        | 0.13          |
| (1,67)  | 1:4:A:TYR:HB2 | 1:7:A:LEU:HD21 | 7        | 0.13          |
| (1,67)  | 1:4:A:TYR:HB2 | 1:7:A:LEU:HD22 | 7        | 0.13          |
| (1,67)  | 1:4:A:TYR:HB2 | 1:7:A:LEU:HD23 | 7        | 0.13          |
| (1,67)  | 1:4:A:TYR:HB3 | 1:7:A:LEU:HD11 | 7        | 0.13          |
| (1,67)  | 1:4:A:TYR:HB3 | 1:7:A:LEU:HD12 | 7        | 0.13          |
| (1,67)  | 1:4:A:TYR:HB3 | 1:7:A:LEU:HD13 | 7        | 0.13          |
| (1,67)  | 1:4:A:TYR:HB3 | 1:7:A:LEU:HD21 | 7        | 0.13          |
| (1,67)  | 1:4:A:TYR:HB3 | 1:7:A:LEU:HD22 | 7        | 0.13          |
| (1,67)  | 1:4:A:TYR:HB3 | 1:7:A:LEU:HD23 | 7        | 0.13          |
| (1,67)  | 1:4:A:TYR:HB2 | 1:7:A:LEU:HD11 | 8        | 0.13          |
| (1,67)  | 1:4:A:TYR:HB2 | 1:7:A:LEU:HD12 | 8        | 0.13          |
| (1,67)  | 1:4:A:TYR:HB2 | 1:7:A:LEU:HD13 | 8        | 0.13          |
| (1,67)  | 1:4:A:TYR:HB2 | 1:7:A:LEU:HD21 | 8        | 0.13          |
| (1,67)  | 1:4:A:TYR:HB2 | 1:7:A:LEU:HD22 | 8        | 0.13          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD23 | 8        | 0.13          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD11 | 8        | 0.13          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD12 | 8        | 0.13          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD13 | 8        | 0.13          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD21 | 8        | 0.13          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD22 | 8        | 0.13          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD23 | 8        | 0.13          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD11 | 13       | 0.13          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD12 | 13       | 0.13          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD13 | 13       | 0.13          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD21 | 13       | 0.13          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD22 | 13       | 0.13          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD23 | 13       | 0.13          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD11 | 13       | 0.13          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD12 | 13       | 0.13          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD13 | 13       | 0.13          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD21 | 13       | 0.13          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD22 | 13       | 0.13          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD23 | 13       | 0.13          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD11 | 19       | 0.13          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD12 | 19       | 0.13          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD13 | 19       | 0.13          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD21 | 19       | 0.13          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD22 | 19       | 0.13          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD23 | 19       | 0.13          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD11 | 19       | 0.13          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD12 | 19       | 0.13          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD13 | 19       | 0.13          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD21 | 19       | 0.13          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD22 | 19       | 0.13          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD23 | 19       | 0.13          |
| (1,20)   | 1:2:A:ALA:HA    | 1:5:A:GLY:H    | 18       | 0.13          |
| (1,20)   | 1:2:A:ALA:HA    | 1:5:A:GLY:H    | 20       | 0.13          |
| (1,10)   | 1:1:A:MET:HA    | 1:57:A:LYS:HD2 | 10       | 0.13          |
| (1,10)   | 1:1:A:MET:HA    | 1:57:A:LYS:HD3 | 10       | 0.13          |
| (1,6)    | 1:1:A:MET:HA    | 1:3:A:GLU:H    | 6        | 0.13          |
| (1,1900) | 1:89:A:ILE:HG21 | 1:90:A:SER:HB2 | 1        | 0.12          |
| (1,1900) | 1:89:A:ILE:HG21 | 1:90:A:SER:HB3 | 1        | 0.12          |
| (1,1900) | 1:89:A:ILE:HG22 | 1:90:A:SER:HB2 | 1        | 0.12          |
| (1,1900) | 1:89:A:ILE:HG22 | 1:90:A:SER:HB3 | 1        | 0.12          |
| (1,1900) | 1:89:A:ILE:HG23 | 1:90:A:SER:HB2 | 1        | 0.12          |
| (1,1900) | 1:89:A:ILE:HG23 | 1:90:A:SER:HB3 | 1        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1900) | 1:89:A:ILE:HG21 | 1:90:A:SER:HB2  | 15       | 0.12          |
| (1,1900) | 1:89:A:ILE:HG21 | 1:90:A:SER:HB3  | 15       | 0.12          |
| (1,1900) | 1:89:A:ILE:HG22 | 1:90:A:SER:HB2  | 15       | 0.12          |
| (1,1900) | 1:89:A:ILE:HG22 | 1:90:A:SER:HB3  | 15       | 0.12          |
| (1,1900) | 1:89:A:ILE:HG23 | 1:90:A:SER:HB2  | 15       | 0.12          |
| (1,1900) | 1:89:A:ILE:HG23 | 1:90:A:SER:HB3  | 15       | 0.12          |
| (1,1900) | 1:89:A:ILE:HG21 | 1:90:A:SER:HB2  | 18       | 0.12          |
| (1,1900) | 1:89:A:ILE:HG21 | 1:90:A:SER:HB3  | 18       | 0.12          |
| (1,1900) | 1:89:A:ILE:HG22 | 1:90:A:SER:HB2  | 18       | 0.12          |
| (1,1900) | 1:89:A:ILE:HG22 | 1:90:A:SER:HB3  | 18       | 0.12          |
| (1,1900) | 1:89:A:ILE:HG23 | 1:90:A:SER:HB2  | 18       | 0.12          |
| (1,1900) | 1:89:A:ILE:HG23 | 1:90:A:SER:HB3  | 18       | 0.12          |
| (1,1900) | 1:89:A:ILE:HG21 | 1:90:A:SER:HB2  | 19       | 0.12          |
| (1,1900) | 1:89:A:ILE:HG21 | 1:90:A:SER:HB3  | 19       | 0.12          |
| (1,1900) | 1:89:A:ILE:HG22 | 1:90:A:SER:HB2  | 19       | 0.12          |
| (1,1900) | 1:89:A:ILE:HG22 | 1:90:A:SER:HB3  | 19       | 0.12          |
| (1,1900) | 1:89:A:ILE:HG23 | 1:90:A:SER:HB2  | 19       | 0.12          |
| (1,1900) | 1:89:A:ILE:HG23 | 1:90:A:SER:HB3  | 19       | 0.12          |
| (1,1888) | 1:89:A:ILE:HG21 | 1:89:A:ILE:H    | 19       | 0.12          |
| (1,1888) | 1:89:A:ILE:HG22 | 1:89:A:ILE:H    | 19       | 0.12          |
| (1,1888) | 1:89:A:ILE:HG23 | 1:89:A:ILE:H    | 19       | 0.12          |
| (1,1885) | 1:88:A:LYS:HG2  | 1:89:A:ILE:HB   | 9        | 0.12          |
| (1,1885) | 1:88:A:LYS:HG3  | 1:89:A:ILE:HB   | 9        | 0.12          |
| (1,1838) | 1:85:A:ARG:H    | 1:86:A:VAL:HB   | 19       | 0.12          |
| (1,1834) | 1:85:A:ARG:HD2  | 1:86:A:VAL:HA   | 3        | 0.12          |
| (1,1834) | 1:85:A:ARG:HD3  | 1:86:A:VAL:HA   | 3        | 0.12          |
| (1,1834) | 1:85:A:ARG:HD2  | 1:86:A:VAL:HA   | 10       | 0.12          |
| (1,1834) | 1:85:A:ARG:HD3  | 1:86:A:VAL:HA   | 10       | 0.12          |
| (1,1834) | 1:85:A:ARG:HD2  | 1:86:A:VAL:HA   | 18       | 0.12          |
| (1,1834) | 1:85:A:ARG:HD3  | 1:86:A:VAL:HA   | 18       | 0.12          |
| (1,1834) | 1:85:A:ARG:HD2  | 1:86:A:VAL:HA   | 19       | 0.12          |
| (1,1834) | 1:85:A:ARG:HD3  | 1:86:A:VAL:HA   | 19       | 0.12          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD11 | 1        | 0.12          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD12 | 1        | 0.12          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD13 | 1        | 0.12          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD21 | 1        | 0.12          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD22 | 1        | 0.12          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD23 | 1        | 0.12          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD11 | 8        | 0.12          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD12 | 8        | 0.12          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD13 | 8        | 0.12          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD21 | 8        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD22 | 8        | 0.12          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD23 | 8        | 0.12          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD11 | 18       | 0.12          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD12 | 18       | 0.12          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD13 | 18       | 0.12          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD21 | 18       | 0.12          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD22 | 18       | 0.12          |
| (1,1822) | 1:84:A:THR:HB   | 1:87:A:LEU:HD23 | 18       | 0.12          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD2  | 3        | 0.12          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD3  | 3        | 0.12          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD2  | 3        | 0.12          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD3  | 3        | 0.12          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD2  | 3        | 0.12          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD3  | 3        | 0.12          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD2  | 18       | 0.12          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD3  | 18       | 0.12          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD2  | 18       | 0.12          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD3  | 18       | 0.12          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD2  | 18       | 0.12          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD3  | 18       | 0.12          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD11 | 9        | 0.12          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD12 | 9        | 0.12          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD13 | 9        | 0.12          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD21 | 9        | 0.12          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD22 | 9        | 0.12          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD23 | 9        | 0.12          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD11 | 9        | 0.12          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD12 | 9        | 0.12          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD13 | 9        | 0.12          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD21 | 9        | 0.12          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD22 | 9        | 0.12          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD23 | 9        | 0.12          |
| (1,1796) | 1:83:A:ARG:HD2  | 1:84:A:THR:HG21 | 17       | 0.12          |
| (1,1796) | 1:83:A:ARG:HD2  | 1:84:A:THR:HG22 | 17       | 0.12          |
| (1,1796) | 1:83:A:ARG:HD2  | 1:84:A:THR:HG23 | 17       | 0.12          |
| (1,1796) | 1:83:A:ARG:HD3  | 1:84:A:THR:HG21 | 17       | 0.12          |
| (1,1796) | 1:83:A:ARG:HD3  | 1:84:A:THR:HG22 | 17       | 0.12          |
| (1,1796) | 1:83:A:ARG:HD3  | 1:84:A:THR:HG23 | 17       | 0.12          |
| (1,1794) | 1:83:A:ARG:HG2  | 1:84:A:THR:H    | 3        | 0.12          |
| (1,1794) | 1:83:A:ARG:HG3  | 1:84:A:THR:H    | 3        | 0.12          |
| (1,1794) | 1:83:A:ARG:HG2  | 1:84:A:THR:H    | 4        | 0.12          |
| (1,1794) | 1:83:A:ARG:HG3  | 1:84:A:THR:H    | 4        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1794) | 1:83:A:ARG:HG2  | 1:84:A:THR:H    | 19       | 0.12          |
| (1,1794) | 1:83:A:ARG:HG3  | 1:84:A:THR:H    | 19       | 0.12          |
| (1,1777) | 1:82:A:TYR:HD1  | 1:85:A:ARG:HG2  | 6        | 0.12          |
| (1,1777) | 1:82:A:TYR:HD1  | 1:85:A:ARG:HG3  | 6        | 0.12          |
| (1,1777) | 1:82:A:TYR:HD2  | 1:85:A:ARG:HG2  | 6        | 0.12          |
| (1,1777) | 1:82:A:TYR:HD2  | 1:85:A:ARG:HG3  | 6        | 0.12          |
| (1,1762) | 1:82:A:TYR:HE1  | 1:82:A:TYR:H    | 15       | 0.12          |
| (1,1762) | 1:82:A:TYR:HE2  | 1:82:A:TYR:H    | 15       | 0.12          |
| (1,1745) | 1:80:A:VAL:HA   | 1:83:A:ARG:HD2  | 16       | 0.12          |
| (1,1745) | 1:80:A:VAL:HA   | 1:83:A:ARG:HD3  | 16       | 0.12          |
| (1,1735) | 1:80:A:VAL:HG11 | 1:81:A:ASP:HA   | 14       | 0.12          |
| (1,1735) | 1:80:A:VAL:HG12 | 1:81:A:ASP:HA   | 14       | 0.12          |
| (1,1735) | 1:80:A:VAL:HG13 | 1:81:A:ASP:HA   | 14       | 0.12          |
| (1,1735) | 1:80:A:VAL:HG21 | 1:81:A:ASP:HA   | 14       | 0.12          |
| (1,1735) | 1:80:A:VAL:HG22 | 1:81:A:ASP:HA   | 14       | 0.12          |
| (1,1735) | 1:80:A:VAL:HG23 | 1:81:A:ASP:HA   | 14       | 0.12          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG11 | 4        | 0.12          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG12 | 4        | 0.12          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG13 | 4        | 0.12          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG21 | 4        | 0.12          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG22 | 4        | 0.12          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG23 | 4        | 0.12          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG11 | 7        | 0.12          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG12 | 7        | 0.12          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG13 | 7        | 0.12          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG21 | 7        | 0.12          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG22 | 7        | 0.12          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG23 | 7        | 0.12          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG11 | 8        | 0.12          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG12 | 8        | 0.12          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG13 | 8        | 0.12          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG21 | 8        | 0.12          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG22 | 8        | 0.12          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG23 | 8        | 0.12          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG11 | 15       | 0.12          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG12 | 15       | 0.12          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG13 | 15       | 0.12          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG21 | 15       | 0.12          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG22 | 15       | 0.12          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG23 | 15       | 0.12          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG11 | 17       | 0.12          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG12 | 17       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG13 | 17       | 0.12          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG21 | 17       | 0.12          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG22 | 17       | 0.12          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG23 | 17       | 0.12          |
| (1,1680) | 1:77:A:THR:HG21 | 1:78:A:MET:HG2  | 10       | 0.12          |
| (1,1680) | 1:77:A:THR:HG21 | 1:78:A:MET:HG3  | 10       | 0.12          |
| (1,1680) | 1:77:A:THR:HG22 | 1:78:A:MET:HG2  | 10       | 0.12          |
| (1,1680) | 1:77:A:THR:HG22 | 1:78:A:MET:HG3  | 10       | 0.12          |
| (1,1680) | 1:77:A:THR:HG23 | 1:78:A:MET:HG2  | 10       | 0.12          |
| (1,1680) | 1:77:A:THR:HG23 | 1:78:A:MET:HG3  | 10       | 0.12          |
| (1,1609) | 1:73:A:PRO:HA   | 1:73:A:PRO:HG2  | 10       | 0.12          |
| (1,1609) | 1:73:A:PRO:HA   | 1:73:A:PRO:HG3  | 10       | 0.12          |
| (1,1609) | 1:73:A:PRO:HA   | 1:73:A:PRO:HG2  | 11       | 0.12          |
| (1,1609) | 1:73:A:PRO:HA   | 1:73:A:PRO:HG3  | 11       | 0.12          |
| (1,1598) | 1:72:A:ARG:HE   | 1:74:A:ASP:H    | 3        | 0.12          |
| (1,1597) | 1:72:A:ARG:HG2  | 1:74:A:ASP:H    | 5        | 0.12          |
| (1,1597) | 1:72:A:ARG:HG3  | 1:74:A:ASP:H    | 5        | 0.12          |
| (1,1588) | 1:72:A:ARG:HA   | 1:72:A:ARG:HE   | 2        | 0.12          |
| (1,1576) | 1:71:A:ARG:HA   | 1:71:A:ARG:HG2  | 4        | 0.12          |
| (1,1576) | 1:71:A:ARG:HA   | 1:71:A:ARG:HG3  | 4        | 0.12          |
| (1,1576) | 1:71:A:ARG:HA   | 1:71:A:ARG:HG2  | 19       | 0.12          |
| (1,1576) | 1:71:A:ARG:HA   | 1:71:A:ARG:HG3  | 19       | 0.12          |
| (1,1538) | 1:68:A:GLU:HA   | 1:71:A:ARG:HD2  | 18       | 0.12          |
| (1,1538) | 1:68:A:GLU:HA   | 1:71:A:ARG:HD3  | 18       | 0.12          |
| (1,1516) | 1:67:A:PHE:H    | 1:76:A:LEU:HG   | 7        | 0.12          |
| (1,1516) | 1:67:A:PHE:H    | 1:76:A:LEU:HG   | 19       | 0.12          |
| (1,1465) | 1:66:A:ILE:HD11 | 1:69:A:ILE:HA   | 15       | 0.12          |
| (1,1465) | 1:66:A:ILE:HD12 | 1:69:A:ILE:HA   | 15       | 0.12          |
| (1,1465) | 1:66:A:ILE:HD13 | 1:69:A:ILE:HA   | 15       | 0.12          |
| (1,1439) | 1:65:A:HIS:HA   | 1:69:A:ILE:H    | 14       | 0.12          |
| (1,1439) | 1:65:A:HIS:HA   | 1:69:A:ILE:H    | 19       | 0.12          |
| (1,1437) | 1:65:A:HIS:HA   | 1:68:A:GLU:H    | 13       | 0.12          |
| (1,1355) | 1:63:A:ILE:HB   | 1:63:A:ILE:H    | 3        | 0.12          |
| (1,1349) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HD11 | 14       | 0.12          |
| (1,1349) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HD12 | 14       | 0.12          |
| (1,1349) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HD13 | 14       | 0.12          |
| (1,1349) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HD11 | 14       | 0.12          |
| (1,1349) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HD12 | 14       | 0.12          |
| (1,1349) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HD13 | 14       | 0.12          |
| (1,1349) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HD11 | 19       | 0.12          |
| (1,1349) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HD12 | 19       | 0.12          |
| (1,1349) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HD13 | 19       | 0.12          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1349) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HD11 | 19       | 0.12          |
| (1,1349) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HD12 | 19       | 0.12          |
| (1,1349) | 1:62:A:TYR:HE2 | 1:66:A:ILE:HD13 | 19       | 0.12          |
| (1,1346) | 1:62:A:TYR:H   | 1:66:A:ILE:HD11 | 16       | 0.12          |
| (1,1346) | 1:62:A:TYR:H   | 1:66:A:ILE:HD12 | 16       | 0.12          |
| (1,1346) | 1:62:A:TYR:H   | 1:66:A:ILE:HD13 | 16       | 0.12          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG21 | 7        | 0.12          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG22 | 7        | 0.12          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG23 | 7        | 0.12          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG21 | 8        | 0.12          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG22 | 8        | 0.12          |
| (1,1319) | 1:61:A:SER:HA  | 1:63:A:ILE:HG23 | 8        | 0.12          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD11 | 5        | 0.12          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD12 | 5        | 0.12          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD13 | 5        | 0.12          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD21 | 5        | 0.12          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD22 | 5        | 0.12          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD23 | 5        | 0.12          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD11 | 7        | 0.12          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD12 | 7        | 0.12          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD13 | 7        | 0.12          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD21 | 7        | 0.12          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD22 | 7        | 0.12          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD23 | 7        | 0.12          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD11 | 10       | 0.12          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD12 | 10       | 0.12          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD13 | 10       | 0.12          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD21 | 10       | 0.12          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD22 | 10       | 0.12          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD23 | 10       | 0.12          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD11 | 12       | 0.12          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD12 | 12       | 0.12          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD13 | 12       | 0.12          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD21 | 12       | 0.12          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD22 | 12       | 0.12          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD23 | 12       | 0.12          |
| (1,1277) | 1:58:A:ASP:H   | 1:60:A:LEU:H    | 16       | 0.12          |
| (1,1277) | 1:58:A:ASP:H   | 1:60:A:LEU:H    | 18       | 0.12          |
| (1,1273) | 1:58:A:ASP:HA  | 1:59:A:ASN:HD21 | 10       | 0.12          |
| (1,1273) | 1:58:A:ASP:HA  | 1:59:A:ASN:HD22 | 10       | 0.12          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD2  | 9        | 0.12          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD3  | 9        | 0.12          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG2  | 5        | 0.12          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG3  | 5        | 0.12          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG2  | 9        | 0.12          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG3  | 9        | 0.12          |
| (1,1233) | 1:55:A:LEU:HG  | 1:63:A:ILE:HB   | 4        | 0.12          |
| (1,1228) | 1:55:A:LEU:HG  | 1:59:A:ASN:HD21 | 1        | 0.12          |
| (1,1228) | 1:55:A:LEU:HG  | 1:59:A:ASN:HD22 | 1        | 0.12          |
| (1,1228) | 1:55:A:LEU:HG  | 1:59:A:ASN:HD21 | 6        | 0.12          |
| (1,1228) | 1:55:A:LEU:HG  | 1:59:A:ASN:HD22 | 6        | 0.12          |
| (1,1223) | 1:55:A:LEU:HG  | 1:56:A:ASP:HA   | 13       | 0.12          |
| (1,1223) | 1:55:A:LEU:HG  | 1:56:A:ASP:HA   | 14       | 0.12          |
| (1,1223) | 1:55:A:LEU:HG  | 1:56:A:ASP:HA   | 18       | 0.12          |
| (1,1223) | 1:55:A:LEU:HG  | 1:56:A:ASP:HA   | 19       | 0.12          |
| (1,1207) | 1:54:A:LYS:HG2 | 1:62:A:TYR:HE1  | 20       | 0.12          |
| (1,1207) | 1:54:A:LYS:HG2 | 1:62:A:TYR:HE2  | 20       | 0.12          |
| (1,1207) | 1:54:A:LYS:HG3 | 1:62:A:TYR:HE1  | 20       | 0.12          |
| (1,1207) | 1:54:A:LYS:HG3 | 1:62:A:TYR:HE2  | 20       | 0.12          |
| (1,1206) | 1:54:A:LYS:HB2 | 1:62:A:TYR:HE1  | 10       | 0.12          |
| (1,1206) | 1:54:A:LYS:HB2 | 1:62:A:TYR:HE2  | 10       | 0.12          |
| (1,1206) | 1:54:A:LYS:HB3 | 1:62:A:TYR:HE1  | 10       | 0.12          |
| (1,1206) | 1:54:A:LYS:HB3 | 1:62:A:TYR:HE2  | 10       | 0.12          |
| (1,1129) | 1:49:A:LEU:HG  | 1:62:A:TYR:HD1  | 7        | 0.12          |
| (1,1129) | 1:49:A:LEU:HG  | 1:62:A:TYR:HD2  | 7        | 0.12          |
| (1,1129) | 1:49:A:LEU:HG  | 1:62:A:TYR:HD1  | 8        | 0.12          |
| (1,1129) | 1:49:A:LEU:HG  | 1:62:A:TYR:HD2  | 8        | 0.12          |
| (1,1062) | 1:47:A:SER:HA  | 1:51:A:SER:H    | 2        | 0.12          |
| (1,1062) | 1:47:A:SER:HA  | 1:51:A:SER:H    | 8        | 0.12          |
| (1,1062) | 1:47:A:SER:HA  | 1:51:A:SER:H    | 11       | 0.12          |
| (1,1062) | 1:47:A:SER:HA  | 1:51:A:SER:H    | 17       | 0.12          |
| (1,1062) | 1:47:A:SER:HA  | 1:51:A:SER:H    | 20       | 0.12          |
| (1,1018) | 1:46:A:PHE:HD1 | 1:46:A:PHE:H    | 19       | 0.12          |
| (1,1018) | 1:46:A:PHE:HD2 | 1:46:A:PHE:H    | 19       | 0.12          |
| (1,1010) | 1:45:A:TRP:HE1 | 1:66:A:ILE:HG12 | 2        | 0.12          |
| (1,1010) | 1:45:A:TRP:HE1 | 1:66:A:ILE:HG13 | 2        | 0.12          |
| (1,1010) | 1:45:A:TRP:HE1 | 1:66:A:ILE:HG12 | 5        | 0.12          |
| (1,1010) | 1:45:A:TRP:HE1 | 1:66:A:ILE:HG13 | 5        | 0.12          |
| (1,997)  | 1:45:A:TRP:HA  | 1:50:A:GLU:H    | 15       | 0.12          |
| (1,982)  | 1:45:A:TRP:HE1 | 1:46:A:PHE:HA   | 7        | 0.12          |
| (1,982)  | 1:45:A:TRP:HE1 | 1:46:A:PHE:HA   | 16       | 0.12          |
| (1,926)  | 1:41:A:THR:HB  | 1:42:A:GLY:H    | 4        | 0.12          |
| (1,926)  | 1:41:A:THR:HB  | 1:42:A:GLY:H    | 11       | 0.12          |
| (1,926)  | 1:41:A:THR:HB  | 1:42:A:GLY:H    | 12       | 0.12          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,926) | 1:41:A:THR:HB  | 1:42:A:GLY:H    | 13       | 0.12          |
| (1,926) | 1:41:A:THR:HB  | 1:42:A:GLY:H    | 17       | 0.12          |
| (1,923) | 1:41:A:THR:HB  | 1:41:A:THR:H    | 7        | 0.12          |
| (1,918) | 1:40:A:THR:HA  | 1:41:A:THR:H    | 2        | 0.12          |
| (1,855) | 1:38:A:GLU:HG2 | 1:39:A:ILE:HD11 | 12       | 0.12          |
| (1,855) | 1:38:A:GLU:HG2 | 1:39:A:ILE:HD12 | 12       | 0.12          |
| (1,855) | 1:38:A:GLU:HG2 | 1:39:A:ILE:HD13 | 12       | 0.12          |
| (1,855) | 1:38:A:GLU:HG3 | 1:39:A:ILE:HD11 | 12       | 0.12          |
| (1,855) | 1:38:A:GLU:HG3 | 1:39:A:ILE:HD12 | 12       | 0.12          |
| (1,855) | 1:38:A:GLU:HG3 | 1:39:A:ILE:HD13 | 12       | 0.12          |
| (1,855) | 1:38:A:GLU:HG2 | 1:39:A:ILE:HD11 | 13       | 0.12          |
| (1,855) | 1:38:A:GLU:HG2 | 1:39:A:ILE:HD12 | 13       | 0.12          |
| (1,855) | 1:38:A:GLU:HG2 | 1:39:A:ILE:HD13 | 13       | 0.12          |
| (1,855) | 1:38:A:GLU:HG3 | 1:39:A:ILE:HD11 | 13       | 0.12          |
| (1,855) | 1:38:A:GLU:HG3 | 1:39:A:ILE:HD12 | 13       | 0.12          |
| (1,855) | 1:38:A:GLU:HG3 | 1:39:A:ILE:HD13 | 13       | 0.12          |
| (1,855) | 1:38:A:GLU:HG2 | 1:39:A:ILE:HD11 | 18       | 0.12          |
| (1,855) | 1:38:A:GLU:HG2 | 1:39:A:ILE:HD12 | 18       | 0.12          |
| (1,855) | 1:38:A:GLU:HG2 | 1:39:A:ILE:HD13 | 18       | 0.12          |
| (1,855) | 1:38:A:GLU:HG3 | 1:39:A:ILE:HD11 | 18       | 0.12          |
| (1,855) | 1:38:A:GLU:HG3 | 1:39:A:ILE:HD12 | 18       | 0.12          |
| (1,855) | 1:38:A:GLU:HG3 | 1:39:A:ILE:HD13 | 18       | 0.12          |
| (1,849) | 1:38:A:GLU:HA  | 1:38:A:GLU:HG2  | 8        | 0.12          |
| (1,849) | 1:38:A:GLU:HA  | 1:38:A:GLU:HG3  | 8        | 0.12          |
| (1,838) | 1:36:A:SER:HA  | 1:39:A:ILE:HD11 | 1        | 0.12          |
| (1,838) | 1:36:A:SER:HA  | 1:39:A:ILE:HD12 | 1        | 0.12          |
| (1,838) | 1:36:A:SER:HA  | 1:39:A:ILE:HD13 | 1        | 0.12          |
| (1,838) | 1:36:A:SER:HA  | 1:39:A:ILE:HD11 | 20       | 0.12          |
| (1,838) | 1:36:A:SER:HA  | 1:39:A:ILE:HD12 | 20       | 0.12          |
| (1,838) | 1:36:A:SER:HA  | 1:39:A:ILE:HD13 | 20       | 0.12          |
| (1,803) | 1:35:A:LYS:HA  | 1:35:A:LYS:HG2  | 8        | 0.12          |
| (1,803) | 1:35:A:LYS:HA  | 1:35:A:LYS:HG3  | 8        | 0.12          |
| (1,783) | 1:32:A:PRO:HD2 | 1:35:A:LYS:HG2  | 8        | 0.12          |
| (1,783) | 1:32:A:PRO:HD2 | 1:35:A:LYS:HG3  | 8        | 0.12          |
| (1,783) | 1:32:A:PRO:HD3 | 1:35:A:LYS:HG2  | 8        | 0.12          |
| (1,783) | 1:32:A:PRO:HD3 | 1:35:A:LYS:HG3  | 8        | 0.12          |
| (1,783) | 1:32:A:PRO:HD2 | 1:35:A:LYS:HG2  | 11       | 0.12          |
| (1,783) | 1:32:A:PRO:HD2 | 1:35:A:LYS:HG3  | 11       | 0.12          |
| (1,783) | 1:32:A:PRO:HD3 | 1:35:A:LYS:HG2  | 11       | 0.12          |
| (1,783) | 1:32:A:PRO:HD3 | 1:35:A:LYS:HG3  | 11       | 0.12          |
| (1,775) | 1:32:A:PRO:HA  | 1:32:A:PRO:HG2  | 4        | 0.12          |
| (1,775) | 1:32:A:PRO:HA  | 1:32:A:PRO:HG3  | 4        | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,775) | 1:32:A:PRO:HA   | 1:32:A:PRO:HG2  | 6        | 0.12          |
| (1,775) | 1:32:A:PRO:HA   | 1:32:A:PRO:HG3  | 6        | 0.12          |
| (1,772) | 1:31:A:ILE:HG21 | 1:49:A:LEU:HA   | 15       | 0.12          |
| (1,772) | 1:31:A:ILE:HG22 | 1:49:A:LEU:HA   | 15       | 0.12          |
| (1,772) | 1:31:A:ILE:HG23 | 1:49:A:LEU:HA   | 15       | 0.12          |
| (1,761) | 1:31:A:ILE:HD11 | 1:45:A:TRP:HD1  | 6        | 0.12          |
| (1,761) | 1:31:A:ILE:HD12 | 1:45:A:TRP:HD1  | 6        | 0.12          |
| (1,761) | 1:31:A:ILE:HD13 | 1:45:A:TRP:HD1  | 6        | 0.12          |
| (1,761) | 1:31:A:ILE:HD11 | 1:45:A:TRP:HD1  | 12       | 0.12          |
| (1,761) | 1:31:A:ILE:HD12 | 1:45:A:TRP:HD1  | 12       | 0.12          |
| (1,761) | 1:31:A:ILE:HD13 | 1:45:A:TRP:HD1  | 12       | 0.12          |
| (1,761) | 1:31:A:ILE:HD11 | 1:45:A:TRP:HD1  | 16       | 0.12          |
| (1,761) | 1:31:A:ILE:HD12 | 1:45:A:TRP:HD1  | 16       | 0.12          |
| (1,761) | 1:31:A:ILE:HD13 | 1:45:A:TRP:HD1  | 16       | 0.12          |
| (1,743) | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD2  | 4        | 0.12          |
| (1,743) | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD3  | 4        | 0.12          |
| (1,743) | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD2  | 4        | 0.12          |
| (1,743) | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD3  | 4        | 0.12          |
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD2  | 4        | 0.12          |
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD3  | 4        | 0.12          |
| (1,736) | 1:31:A:ILE:HB   | 1:32:A:PRO:HA   | 2        | 0.12          |
| (1,736) | 1:31:A:ILE:HB   | 1:32:A:PRO:HA   | 5        | 0.12          |
| (1,736) | 1:31:A:ILE:HB   | 1:32:A:PRO:HA   | 15       | 0.12          |
| (1,736) | 1:31:A:ILE:HB   | 1:32:A:PRO:HA   | 17       | 0.12          |
| (1,724) | 1:31:A:ILE:HD11 | 1:31:A:ILE:H    | 11       | 0.12          |
| (1,724) | 1:31:A:ILE:HD12 | 1:31:A:ILE:H    | 11       | 0.12          |
| (1,724) | 1:31:A:ILE:HD13 | 1:31:A:ILE:H    | 11       | 0.12          |
| (1,724) | 1:31:A:ILE:HD11 | 1:31:A:ILE:H    | 16       | 0.12          |
| (1,724) | 1:31:A:ILE:HD12 | 1:31:A:ILE:H    | 16       | 0.12          |
| (1,724) | 1:31:A:ILE:HD13 | 1:31:A:ILE:H    | 16       | 0.12          |
| (1,669) | 1:27:A:CYS:HB2  | 1:30:A:ASP:H    | 16       | 0.12          |
| (1,669) | 1:27:A:CYS:HB3  | 1:30:A:ASP:H    | 16       | 0.12          |
| (1,633) | 1:25:A:SER:HA   | 1:28:A:LYS:H    | 13       | 0.12          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG21 | 7        | 0.12          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG22 | 7        | 0.12          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG23 | 7        | 0.12          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG21 | 18       | 0.12          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG22 | 18       | 0.12          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG23 | 18       | 0.12          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG21 | 20       | 0.12          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG22 | 20       | 0.12          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG23 | 20       | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,555) | 1:22:A:GLN:HA   | 1:23:A:LEU:H    | 6        | 0.12          |
| (1,555) | 1:22:A:GLN:HA   | 1:23:A:LEU:H    | 8        | 0.12          |
| (1,555) | 1:22:A:GLN:HA   | 1:23:A:LEU:H    | 9        | 0.12          |
| (1,555) | 1:22:A:GLN:HA   | 1:23:A:LEU:H    | 12       | 0.12          |
| (1,555) | 1:22:A:GLN:HA   | 1:23:A:LEU:H    | 16       | 0.12          |
| (1,555) | 1:22:A:GLN:HA   | 1:23:A:LEU:H    | 18       | 0.12          |
| (1,555) | 1:22:A:GLN:HA   | 1:23:A:LEU:H    | 20       | 0.12          |
| (1,537) | 1:21:A:GLU:HA   | 1:21:A:GLU:HG2  | 5        | 0.12          |
| (1,537) | 1:21:A:GLU:HA   | 1:21:A:GLU:HG3  | 5        | 0.12          |
| (1,534) | 1:20:A:LEU:HD11 | 1:67:A:PHE:HE1  | 18       | 0.12          |
| (1,534) | 1:20:A:LEU:HD11 | 1:67:A:PHE:HE2  | 18       | 0.12          |
| (1,534) | 1:20:A:LEU:HD12 | 1:67:A:PHE:HE1  | 18       | 0.12          |
| (1,534) | 1:20:A:LEU:HD12 | 1:67:A:PHE:HE2  | 18       | 0.12          |
| (1,534) | 1:20:A:LEU:HD13 | 1:67:A:PHE:HE1  | 18       | 0.12          |
| (1,534) | 1:20:A:LEU:HD13 | 1:67:A:PHE:HE2  | 18       | 0.12          |
| (1,534) | 1:20:A:LEU:HD21 | 1:67:A:PHE:HE1  | 18       | 0.12          |
| (1,534) | 1:20:A:LEU:HD21 | 1:67:A:PHE:HE2  | 18       | 0.12          |
| (1,534) | 1:20:A:LEU:HD22 | 1:67:A:PHE:HE1  | 18       | 0.12          |
| (1,534) | 1:20:A:LEU:HD22 | 1:67:A:PHE:HE2  | 18       | 0.12          |
| (1,534) | 1:20:A:LEU:HD23 | 1:67:A:PHE:HE1  | 18       | 0.12          |
| (1,534) | 1:20:A:LEU:HD23 | 1:67:A:PHE:HE2  | 18       | 0.12          |
| (1,487) | 1:20:A:LEU:HG   | 1:20:A:LEU:H    | 13       | 0.12          |
| (1,483) | 1:19:A:ASP:HA   | 1:22:A:GLN:HE21 | 10       | 0.12          |
| (1,483) | 1:19:A:ASP:HA   | 1:22:A:GLN:HE22 | 10       | 0.12          |
| (1,480) | 1:19:A:ASP:HA   | 1:22:A:GLN:H    | 18       | 0.12          |
| (1,476) | 1:19:A:ASP:H    | 1:20:A:LEU:H    | 16       | 0.12          |
| (1,461) | 1:17:A:LEU:HD11 | 1:40:A:THR:HG21 | 6        | 0.12          |
| (1,461) | 1:17:A:LEU:HD11 | 1:40:A:THR:HG22 | 6        | 0.12          |
| (1,461) | 1:17:A:LEU:HD11 | 1:40:A:THR:HG23 | 6        | 0.12          |
| (1,461) | 1:17:A:LEU:HD12 | 1:40:A:THR:HG21 | 6        | 0.12          |
| (1,461) | 1:17:A:LEU:HD12 | 1:40:A:THR:HG22 | 6        | 0.12          |
| (1,461) | 1:17:A:LEU:HD12 | 1:40:A:THR:HG23 | 6        | 0.12          |
| (1,461) | 1:17:A:LEU:HD13 | 1:40:A:THR:HG21 | 6        | 0.12          |
| (1,461) | 1:17:A:LEU:HD13 | 1:40:A:THR:HG22 | 6        | 0.12          |
| (1,461) | 1:17:A:LEU:HD13 | 1:40:A:THR:HG23 | 6        | 0.12          |
| (1,461) | 1:17:A:LEU:HD21 | 1:40:A:THR:HG21 | 6        | 0.12          |
| (1,461) | 1:17:A:LEU:HD21 | 1:40:A:THR:HG22 | 6        | 0.12          |
| (1,461) | 1:17:A:LEU:HD21 | 1:40:A:THR:HG23 | 6        | 0.12          |
| (1,461) | 1:17:A:LEU:HD22 | 1:40:A:THR:HG21 | 6        | 0.12          |
| (1,461) | 1:17:A:LEU:HD22 | 1:40:A:THR:HG22 | 6        | 0.12          |
| (1,461) | 1:17:A:LEU:HD22 | 1:40:A:THR:HG23 | 6        | 0.12          |
| (1,461) | 1:17:A:LEU:HD23 | 1:40:A:THR:HG21 | 6        | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,461) | 1:17:A:LEU:HD23 | 1:40:A:THR:HG22 | 6        | 0.12          |
| (1,461) | 1:17:A:LEU:HD23 | 1:40:A:THR:HG23 | 6        | 0.12          |
| (1,459) | 1:17:A:LEU:HG   | 1:40:A:THR:HB   | 11       | 0.12          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB2  | 9        | 0.12          |
| (1,432) | 1:16:A:THR:HG21 | 1:19:A:ASP:HB3  | 9        | 0.12          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB2  | 9        | 0.12          |
| (1,432) | 1:16:A:THR:HG22 | 1:19:A:ASP:HB3  | 9        | 0.12          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB2  | 9        | 0.12          |
| (1,432) | 1:16:A:THR:HG23 | 1:19:A:ASP:HB3  | 9        | 0.12          |
| (1,425) | 1:16:A:THR:HG21 | 1:18:A:GLU:H    | 5        | 0.12          |
| (1,425) | 1:16:A:THR:HG22 | 1:18:A:GLU:H    | 5        | 0.12          |
| (1,425) | 1:16:A:THR:HG23 | 1:18:A:GLU:H    | 5        | 0.12          |
| (1,420) | 1:16:A:THR:HG21 | 1:17:A:LEU:H    | 4        | 0.12          |
| (1,420) | 1:16:A:THR:HG22 | 1:17:A:LEU:H    | 4        | 0.12          |
| (1,420) | 1:16:A:THR:HG23 | 1:17:A:LEU:H    | 4        | 0.12          |
| (1,420) | 1:16:A:THR:HG21 | 1:17:A:LEU:H    | 5        | 0.12          |
| (1,420) | 1:16:A:THR:HG22 | 1:17:A:LEU:H    | 5        | 0.12          |
| (1,420) | 1:16:A:THR:HG23 | 1:17:A:LEU:H    | 5        | 0.12          |
| (1,420) | 1:16:A:THR:HG21 | 1:17:A:LEU:H    | 6        | 0.12          |
| (1,420) | 1:16:A:THR:HG22 | 1:17:A:LEU:H    | 6        | 0.12          |
| (1,420) | 1:16:A:THR:HG23 | 1:17:A:LEU:H    | 6        | 0.12          |
| (1,418) | 1:16:A:THR:HB   | 1:16:A:THR:H    | 2        | 0.12          |
| (1,418) | 1:16:A:THR:HB   | 1:16:A:THR:H    | 14       | 0.12          |
| (1,418) | 1:16:A:THR:HB   | 1:16:A:THR:H    | 15       | 0.12          |
| (1,405) | 1:15:A:ILE:HD11 | 1:43:A:SER:H    | 10       | 0.12          |
| (1,405) | 1:15:A:ILE:HD12 | 1:43:A:SER:H    | 10       | 0.12          |
| (1,405) | 1:15:A:ILE:HD13 | 1:43:A:SER:H    | 10       | 0.12          |
| (1,398) | 1:15:A:ILE:HD11 | 1:23:A:LEU:HB2  | 20       | 0.12          |
| (1,398) | 1:15:A:ILE:HD11 | 1:23:A:LEU:HB3  | 20       | 0.12          |
| (1,398) | 1:15:A:ILE:HD12 | 1:23:A:LEU:HB2  | 20       | 0.12          |
| (1,398) | 1:15:A:ILE:HD12 | 1:23:A:LEU:HB3  | 20       | 0.12          |
| (1,398) | 1:15:A:ILE:HD13 | 1:23:A:LEU:HB2  | 20       | 0.12          |
| (1,398) | 1:15:A:ILE:HD13 | 1:23:A:LEU:HB3  | 20       | 0.12          |
| (1,387) | 1:15:A:ILE:HD11 | 1:19:A:ASP:H    | 8        | 0.12          |
| (1,387) | 1:15:A:ILE:HD12 | 1:19:A:ASP:H    | 8        | 0.12          |
| (1,387) | 1:15:A:ILE:HD13 | 1:19:A:ASP:H    | 8        | 0.12          |
| (1,373) | 1:14:A:ASN:HB2  | 1:75:A:LEU:HG   | 12       | 0.12          |
| (1,373) | 1:14:A:ASN:HB3  | 1:75:A:LEU:HG   | 12       | 0.12          |
| (1,373) | 1:14:A:ASN:HB2  | 1:75:A:LEU:HG   | 14       | 0.12          |
| (1,373) | 1:14:A:ASN:HB3  | 1:75:A:LEU:HG   | 14       | 0.12          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD1  | 16       | 0.12          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD2  | 16       | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD1  | 16       | 0.12          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD2  | 16       | 0.12          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD1  | 16       | 0.12          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD2  | 16       | 0.12          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD1  | 17       | 0.12          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD2  | 17       | 0.12          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD1  | 17       | 0.12          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD2  | 17       | 0.12          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD1  | 17       | 0.12          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD2  | 17       | 0.12          |
| (1,304) | 1:11:A:LEU:HD11 | 1:75:A:LEU:HG   | 14       | 0.12          |
| (1,304) | 1:11:A:LEU:HD12 | 1:75:A:LEU:HG   | 14       | 0.12          |
| (1,304) | 1:11:A:LEU:HD13 | 1:75:A:LEU:HG   | 14       | 0.12          |
| (1,304) | 1:11:A:LEU:HD21 | 1:75:A:LEU:HG   | 14       | 0.12          |
| (1,304) | 1:11:A:LEU:HD22 | 1:75:A:LEU:HG   | 14       | 0.12          |
| (1,304) | 1:11:A:LEU:HD23 | 1:75:A:LEU:HG   | 14       | 0.12          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD11 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD12 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD13 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD21 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD22 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD23 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD11 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD12 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD13 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD21 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD22 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD23 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD11 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD12 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD13 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD21 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD22 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD23 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD11 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD12 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD13 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD21 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD22 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD23 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD11 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD12 | 3        | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD13 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD21 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD22 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD23 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD11 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD12 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD13 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD21 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD22 | 3        | 0.12          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD23 | 3        | 0.12          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG21 | 9        | 0.12          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG22 | 9        | 0.12          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG23 | 9        | 0.12          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG21 | 9        | 0.12          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG22 | 9        | 0.12          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG23 | 9        | 0.12          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG21 | 11       | 0.12          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG22 | 11       | 0.12          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG23 | 11       | 0.12          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG21 | 11       | 0.12          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG22 | 11       | 0.12          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG23 | 11       | 0.12          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG21 | 12       | 0.12          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG22 | 12       | 0.12          |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG23 | 12       | 0.12          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG21 | 12       | 0.12          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG22 | 12       | 0.12          |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG23 | 12       | 0.12          |
| (1,263) | 1:10:A:ASP:H    | 1:14:A:ASN:H    | 3        | 0.12          |
| (1,263) | 1:10:A:ASP:H    | 1:14:A:ASN:H    | 9        | 0.12          |
| (1,263) | 1:10:A:ASP:H    | 1:14:A:ASN:H    | 10       | 0.12          |
| (1,204) | 1:8:A:LEU:HB2   | 1:46:A:PHE:HE1  | 1        | 0.12          |
| (1,204) | 1:8:A:LEU:HB2   | 1:46:A:PHE:HE2  | 1        | 0.12          |
| (1,204) | 1:8:A:LEU:HB3   | 1:46:A:PHE:HE1  | 1        | 0.12          |
| (1,204) | 1:8:A:LEU:HB3   | 1:46:A:PHE:HE2  | 1        | 0.12          |
| (1,204) | 1:8:A:LEU:HB2   | 1:46:A:PHE:HE1  | 5        | 0.12          |
| (1,204) | 1:8:A:LEU:HB2   | 1:46:A:PHE:HE2  | 5        | 0.12          |
| (1,204) | 1:8:A:LEU:HB3   | 1:46:A:PHE:HE1  | 5        | 0.12          |
| (1,204) | 1:8:A:LEU:HB3   | 1:46:A:PHE:HE2  | 5        | 0.12          |
| (1,204) | 1:8:A:LEU:HB2   | 1:46:A:PHE:HE1  | 6        | 0.12          |
| (1,204) | 1:8:A:LEU:HB2   | 1:46:A:PHE:HE2  | 6        | 0.12          |
| (1,204) | 1:8:A:LEU:HB3   | 1:46:A:PHE:HE1  | 6        | 0.12          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,204) | 1:8:A:LEU:HB3  | 1:46:A:PHE:HE2 | 6        | 0.12          |
| (1,204) | 1:8:A:LEU:HB2  | 1:46:A:PHE:HE1 | 9        | 0.12          |
| (1,204) | 1:8:A:LEU:HB2  | 1:46:A:PHE:HE2 | 9        | 0.12          |
| (1,204) | 1:8:A:LEU:HB3  | 1:46:A:PHE:HE1 | 9        | 0.12          |
| (1,204) | 1:8:A:LEU:HB3  | 1:46:A:PHE:HE2 | 9        | 0.12          |
| (1,196) | 1:8:A:LEU:HD11 | 1:11:A:LEU:HB2 | 19       | 0.12          |
| (1,196) | 1:8:A:LEU:HD11 | 1:11:A:LEU:HB3 | 19       | 0.12          |
| (1,196) | 1:8:A:LEU:HD12 | 1:11:A:LEU:HB2 | 19       | 0.12          |
| (1,196) | 1:8:A:LEU:HD12 | 1:11:A:LEU:HB3 | 19       | 0.12          |
| (1,196) | 1:8:A:LEU:HD13 | 1:11:A:LEU:HB2 | 19       | 0.12          |
| (1,196) | 1:8:A:LEU:HD13 | 1:11:A:LEU:HB3 | 19       | 0.12          |
| (1,196) | 1:8:A:LEU:HD21 | 1:11:A:LEU:HB2 | 19       | 0.12          |
| (1,196) | 1:8:A:LEU:HD21 | 1:11:A:LEU:HB3 | 19       | 0.12          |
| (1,196) | 1:8:A:LEU:HD22 | 1:11:A:LEU:HB2 | 19       | 0.12          |
| (1,196) | 1:8:A:LEU:HD22 | 1:11:A:LEU:HB3 | 19       | 0.12          |
| (1,196) | 1:8:A:LEU:HD23 | 1:11:A:LEU:HB2 | 19       | 0.12          |
| (1,196) | 1:8:A:LEU:HD23 | 1:11:A:LEU:HB3 | 19       | 0.12          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD11 | 4        | 0.12          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD12 | 4        | 0.12          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD13 | 4        | 0.12          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD21 | 4        | 0.12          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD22 | 4        | 0.12          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD23 | 4        | 0.12          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD11 | 9        | 0.12          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD12 | 9        | 0.12          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD13 | 9        | 0.12          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD21 | 9        | 0.12          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD22 | 9        | 0.12          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD23 | 9        | 0.12          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD11 | 14       | 0.12          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD12 | 14       | 0.12          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD13 | 14       | 0.12          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD21 | 14       | 0.12          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD22 | 14       | 0.12          |
| (1,147) | 1:7:A:LEU:HG   | 1:8:A:LEU:HD23 | 14       | 0.12          |
| (1,133) | 1:6:A:THR:HG21 | 1:10:A:ASP:HB2 | 15       | 0.12          |
| (1,133) | 1:6:A:THR:HG21 | 1:10:A:ASP:HB3 | 15       | 0.12          |
| (1,133) | 1:6:A:THR:HG22 | 1:10:A:ASP:HB2 | 15       | 0.12          |
| (1,133) | 1:6:A:THR:HG22 | 1:10:A:ASP:HB3 | 15       | 0.12          |
| (1,133) | 1:6:A:THR:HG23 | 1:10:A:ASP:HB2 | 15       | 0.12          |
| (1,133) | 1:6:A:THR:HG23 | 1:10:A:ASP:HB3 | 15       | 0.12          |
| (1,133) | 1:6:A:THR:HG21 | 1:10:A:ASP:HB2 | 20       | 0.12          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,133) | 1:6:A:THR:HG21 | 1:10:A:ASP:HB3 | 20       | 0.12          |
| (1,133) | 1:6:A:THR:HG22 | 1:10:A:ASP:HB2 | 20       | 0.12          |
| (1,133) | 1:6:A:THR:HG22 | 1:10:A:ASP:HB3 | 20       | 0.12          |
| (1,133) | 1:6:A:THR:HG23 | 1:10:A:ASP:HB2 | 20       | 0.12          |
| (1,133) | 1:6:A:THR:HG23 | 1:10:A:ASP:HB3 | 20       | 0.12          |
| (1,127) | 1:6:A:THR:HB   | 1:9:A:GLN:HG2  | 1        | 0.12          |
| (1,127) | 1:6:A:THR:HB   | 1:9:A:GLN:HG3  | 1        | 0.12          |
| (1,127) | 1:6:A:THR:HB   | 1:9:A:GLN:HG2  | 8        | 0.12          |
| (1,127) | 1:6:A:THR:HB   | 1:9:A:GLN:HG3  | 8        | 0.12          |
| (1,127) | 1:6:A:THR:HB   | 1:9:A:GLN:HG2  | 9        | 0.12          |
| (1,127) | 1:6:A:THR:HB   | 1:9:A:GLN:HG3  | 9        | 0.12          |
| (1,127) | 1:6:A:THR:HB   | 1:9:A:GLN:HG2  | 13       | 0.12          |
| (1,127) | 1:6:A:THR:HB   | 1:9:A:GLN:HG3  | 13       | 0.12          |
| (1,127) | 1:6:A:THR:HB   | 1:9:A:GLN:HG2  | 17       | 0.12          |
| (1,127) | 1:6:A:THR:HB   | 1:9:A:GLN:HG3  | 17       | 0.12          |
| (1,124) | 1:6:A:THR:HA   | 1:9:A:GLN:HG2  | 9        | 0.12          |
| (1,124) | 1:6:A:THR:HA   | 1:9:A:GLN:HG3  | 9        | 0.12          |
| (1,93)  | 1:4:A:TYR:HA   | 1:82:A:TYR:HE1 | 15       | 0.12          |
| (1,93)  | 1:4:A:TYR:HA   | 1:82:A:TYR:HE2 | 15       | 0.12          |
| (1,67)  | 1:4:A:TYR:HB2  | 1:7:A:LEU:HD11 | 17       | 0.12          |
| (1,67)  | 1:4:A:TYR:HB2  | 1:7:A:LEU:HD12 | 17       | 0.12          |
| (1,67)  | 1:4:A:TYR:HB2  | 1:7:A:LEU:HD13 | 17       | 0.12          |
| (1,67)  | 1:4:A:TYR:HB2  | 1:7:A:LEU:HD21 | 17       | 0.12          |
| (1,67)  | 1:4:A:TYR:HB2  | 1:7:A:LEU:HD22 | 17       | 0.12          |
| (1,67)  | 1:4:A:TYR:HB2  | 1:7:A:LEU:HD23 | 17       | 0.12          |
| (1,67)  | 1:4:A:TYR:HB3  | 1:7:A:LEU:HD11 | 17       | 0.12          |
| (1,67)  | 1:4:A:TYR:HB3  | 1:7:A:LEU:HD12 | 17       | 0.12          |
| (1,67)  | 1:4:A:TYR:HB3  | 1:7:A:LEU:HD13 | 17       | 0.12          |
| (1,67)  | 1:4:A:TYR:HB3  | 1:7:A:LEU:HD21 | 17       | 0.12          |
| (1,67)  | 1:4:A:TYR:HB3  | 1:7:A:LEU:HD22 | 17       | 0.12          |
| (1,67)  | 1:4:A:TYR:HB3  | 1:7:A:LEU:HD23 | 17       | 0.12          |
| (1,34)  | 1:3:A:GLU:HG2  | 1:82:A:TYR:HD1 | 4        | 0.12          |
| (1,34)  | 1:3:A:GLU:HG2  | 1:82:A:TYR:HD2 | 4        | 0.12          |
| (1,34)  | 1:3:A:GLU:HG3  | 1:82:A:TYR:HD1 | 4        | 0.12          |
| (1,34)  | 1:3:A:GLU:HG3  | 1:82:A:TYR:HD2 | 4        | 0.12          |
| (1,34)  | 1:3:A:GLU:HG2  | 1:82:A:TYR:HD1 | 11       | 0.12          |
| (1,34)  | 1:3:A:GLU:HG2  | 1:82:A:TYR:HD2 | 11       | 0.12          |
| (1,34)  | 1:3:A:GLU:HG3  | 1:82:A:TYR:HD1 | 11       | 0.12          |
| (1,34)  | 1:3:A:GLU:HG3  | 1:82:A:TYR:HD2 | 11       | 0.12          |
| (1,25)  | 1:3:A:GLU:HG2  | 1:3:A:GLU:HA   | 18       | 0.12          |
| (1,25)  | 1:3:A:GLU:HG3  | 1:3:A:GLU:HA   | 18       | 0.12          |
| (1,20)  | 1:2:A:ALA:HA   | 1:5:A:GLY:H    | 10       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,6)    | 1:1:A:MET:HA    | 1:3:A:GLU:H     | 4        | 0.12          |
| (1,1888) | 1:89:A:ILE:HG21 | 1:89:A:ILE:H    | 14       | 0.11          |
| (1,1888) | 1:89:A:ILE:HG22 | 1:89:A:ILE:H    | 14       | 0.11          |
| (1,1888) | 1:89:A:ILE:HG23 | 1:89:A:ILE:H    | 14       | 0.11          |
| (1,1874) | 1:87:A:LEU:HB2  | 1:89:A:ILE:HG21 | 17       | 0.11          |
| (1,1874) | 1:87:A:LEU:HB2  | 1:89:A:ILE:HG22 | 17       | 0.11          |
| (1,1874) | 1:87:A:LEU:HB2  | 1:89:A:ILE:HG23 | 17       | 0.11          |
| (1,1874) | 1:87:A:LEU:HB3  | 1:89:A:ILE:HG21 | 17       | 0.11          |
| (1,1874) | 1:87:A:LEU:HB3  | 1:89:A:ILE:HG22 | 17       | 0.11          |
| (1,1874) | 1:87:A:LEU:HB3  | 1:89:A:ILE:HG23 | 17       | 0.11          |
| (1,1838) | 1:85:A:ARG:H    | 1:86:A:VAL:HB   | 4        | 0.11          |
| (1,1838) | 1:85:A:ARG:H    | 1:86:A:VAL:HB   | 11       | 0.11          |
| (1,1823) | 1:84:A:THR:HB   | 1:87:A:LEU:HB2  | 14       | 0.11          |
| (1,1823) | 1:84:A:THR:HB   | 1:87:A:LEU:HB3  | 14       | 0.11          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD2  | 12       | 0.11          |
| (1,1812) | 1:84:A:THR:HG21 | 1:85:A:ARG:HD3  | 12       | 0.11          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD2  | 12       | 0.11          |
| (1,1812) | 1:84:A:THR:HG22 | 1:85:A:ARG:HD3  | 12       | 0.11          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD2  | 12       | 0.11          |
| (1,1812) | 1:84:A:THR:HG23 | 1:85:A:ARG:HD3  | 12       | 0.11          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD11 | 18       | 0.11          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD12 | 18       | 0.11          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD13 | 18       | 0.11          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD21 | 18       | 0.11          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD22 | 18       | 0.11          |
| (1,1805) | 1:83:A:ARG:HG2  | 1:87:A:LEU:HD23 | 18       | 0.11          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD11 | 18       | 0.11          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD12 | 18       | 0.11          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD13 | 18       | 0.11          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD21 | 18       | 0.11          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD22 | 18       | 0.11          |
| (1,1805) | 1:83:A:ARG:HG3  | 1:87:A:LEU:HD23 | 18       | 0.11          |
| (1,1794) | 1:83:A:ARG:HG2  | 1:84:A:THR:H    | 7        | 0.11          |
| (1,1794) | 1:83:A:ARG:HG3  | 1:84:A:THR:H    | 7        | 0.11          |
| (1,1794) | 1:83:A:ARG:HG2  | 1:84:A:THR:H    | 10       | 0.11          |
| (1,1794) | 1:83:A:ARG:HG3  | 1:84:A:THR:H    | 10       | 0.11          |
| (1,1794) | 1:83:A:ARG:HG2  | 1:84:A:THR:H    | 11       | 0.11          |
| (1,1794) | 1:83:A:ARG:HG3  | 1:84:A:THR:H    | 11       | 0.11          |
| (1,1781) | 1:82:A:TYR:HB2  | 1:86:A:VAL:HG11 | 9        | 0.11          |
| (1,1781) | 1:82:A:TYR:HB2  | 1:86:A:VAL:HG12 | 9        | 0.11          |
| (1,1781) | 1:82:A:TYR:HB2  | 1:86:A:VAL:HG13 | 9        | 0.11          |
| (1,1781) | 1:82:A:TYR:HB2  | 1:86:A:VAL:HG21 | 9        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1781) | 1:82:A:TYR:HB2  | 1:86:A:VAL:HG22 | 9        | 0.11          |
| (1,1781) | 1:82:A:TYR:HB2  | 1:86:A:VAL:HG23 | 9        | 0.11          |
| (1,1781) | 1:82:A:TYR:HB3  | 1:86:A:VAL:HG11 | 9        | 0.11          |
| (1,1781) | 1:82:A:TYR:HB3  | 1:86:A:VAL:HG12 | 9        | 0.11          |
| (1,1781) | 1:82:A:TYR:HB3  | 1:86:A:VAL:HG13 | 9        | 0.11          |
| (1,1781) | 1:82:A:TYR:HB3  | 1:86:A:VAL:HG21 | 9        | 0.11          |
| (1,1781) | 1:82:A:TYR:HB3  | 1:86:A:VAL:HG22 | 9        | 0.11          |
| (1,1781) | 1:82:A:TYR:HB3  | 1:86:A:VAL:HG23 | 9        | 0.11          |
| (1,1781) | 1:82:A:TYR:HB2  | 1:86:A:VAL:HG11 | 15       | 0.11          |
| (1,1781) | 1:82:A:TYR:HB2  | 1:86:A:VAL:HG12 | 15       | 0.11          |
| (1,1781) | 1:82:A:TYR:HB2  | 1:86:A:VAL:HG13 | 15       | 0.11          |
| (1,1781) | 1:82:A:TYR:HB2  | 1:86:A:VAL:HG21 | 15       | 0.11          |
| (1,1781) | 1:82:A:TYR:HB2  | 1:86:A:VAL:HG22 | 15       | 0.11          |
| (1,1781) | 1:82:A:TYR:HB2  | 1:86:A:VAL:HG23 | 15       | 0.11          |
| (1,1781) | 1:82:A:TYR:HB3  | 1:86:A:VAL:HG11 | 15       | 0.11          |
| (1,1781) | 1:82:A:TYR:HB3  | 1:86:A:VAL:HG12 | 15       | 0.11          |
| (1,1781) | 1:82:A:TYR:HB3  | 1:86:A:VAL:HG13 | 15       | 0.11          |
| (1,1781) | 1:82:A:TYR:HB3  | 1:86:A:VAL:HG21 | 15       | 0.11          |
| (1,1781) | 1:82:A:TYR:HB3  | 1:86:A:VAL:HG22 | 15       | 0.11          |
| (1,1781) | 1:82:A:TYR:HB3  | 1:86:A:VAL:HG23 | 15       | 0.11          |
| (1,1777) | 1:82:A:TYR:HD1  | 1:85:A:ARG:HG2  | 17       | 0.11          |
| (1,1777) | 1:82:A:TYR:HD1  | 1:85:A:ARG:HG3  | 17       | 0.11          |
| (1,1777) | 1:82:A:TYR:HD2  | 1:85:A:ARG:HG2  | 17       | 0.11          |
| (1,1777) | 1:82:A:TYR:HD2  | 1:85:A:ARG:HG3  | 17       | 0.11          |
| (1,1777) | 1:82:A:TYR:HD1  | 1:85:A:ARG:HG2  | 20       | 0.11          |
| (1,1777) | 1:82:A:TYR:HD1  | 1:85:A:ARG:HG3  | 20       | 0.11          |
| (1,1777) | 1:82:A:TYR:HD2  | 1:85:A:ARG:HG2  | 20       | 0.11          |
| (1,1777) | 1:82:A:TYR:HD2  | 1:85:A:ARG:HG3  | 20       | 0.11          |
| (1,1762) | 1:82:A:TYR:HE1  | 1:82:A:TYR:H    | 14       | 0.11          |
| (1,1762) | 1:82:A:TYR:HE2  | 1:82:A:TYR:H    | 14       | 0.11          |
| (1,1745) | 1:80:A:VAL:HA   | 1:83:A:ARG:HD2  | 13       | 0.11          |
| (1,1745) | 1:80:A:VAL:HA   | 1:83:A:ARG:HD3  | 13       | 0.11          |
| (1,1735) | 1:80:A:VAL:HG11 | 1:81:A:ASP:HA   | 11       | 0.11          |
| (1,1735) | 1:80:A:VAL:HG12 | 1:81:A:ASP:HA   | 11       | 0.11          |
| (1,1735) | 1:80:A:VAL:HG13 | 1:81:A:ASP:HA   | 11       | 0.11          |
| (1,1735) | 1:80:A:VAL:HG21 | 1:81:A:ASP:HA   | 11       | 0.11          |
| (1,1735) | 1:80:A:VAL:HG22 | 1:81:A:ASP:HA   | 11       | 0.11          |
| (1,1735) | 1:80:A:VAL:HG23 | 1:81:A:ASP:HA   | 11       | 0.11          |
| (1,1690) | 1:77:A:THR:HG21 | 1:80:A:VAL:HG11 | 8        | 0.11          |
| (1,1690) | 1:77:A:THR:HG21 | 1:80:A:VAL:HG12 | 8        | 0.11          |
| (1,1690) | 1:77:A:THR:HG21 | 1:80:A:VAL:HG13 | 8        | 0.11          |
| (1,1690) | 1:77:A:THR:HG21 | 1:80:A:VAL:HG21 | 8        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1690) | 1:77:A:THR:HG21 | 1:80:A:VAL:HG22 | 8        | 0.11          |
| (1,1690) | 1:77:A:THR:HG21 | 1:80:A:VAL:HG23 | 8        | 0.11          |
| (1,1690) | 1:77:A:THR:HG22 | 1:80:A:VAL:HG11 | 8        | 0.11          |
| (1,1690) | 1:77:A:THR:HG22 | 1:80:A:VAL:HG12 | 8        | 0.11          |
| (1,1690) | 1:77:A:THR:HG22 | 1:80:A:VAL:HG13 | 8        | 0.11          |
| (1,1690) | 1:77:A:THR:HG22 | 1:80:A:VAL:HG21 | 8        | 0.11          |
| (1,1690) | 1:77:A:THR:HG22 | 1:80:A:VAL:HG22 | 8        | 0.11          |
| (1,1690) | 1:77:A:THR:HG22 | 1:80:A:VAL:HG23 | 8        | 0.11          |
| (1,1690) | 1:77:A:THR:HG23 | 1:80:A:VAL:HG11 | 8        | 0.11          |
| (1,1690) | 1:77:A:THR:HG23 | 1:80:A:VAL:HG12 | 8        | 0.11          |
| (1,1690) | 1:77:A:THR:HG23 | 1:80:A:VAL:HG13 | 8        | 0.11          |
| (1,1690) | 1:77:A:THR:HG23 | 1:80:A:VAL:HG21 | 8        | 0.11          |
| (1,1690) | 1:77:A:THR:HG23 | 1:80:A:VAL:HG22 | 8        | 0.11          |
| (1,1690) | 1:77:A:THR:HG23 | 1:80:A:VAL:HG23 | 8        | 0.11          |
| (1,1690) | 1:77:A:THR:HG21 | 1:80:A:VAL:HG11 | 15       | 0.11          |
| (1,1690) | 1:77:A:THR:HG21 | 1:80:A:VAL:HG12 | 15       | 0.11          |
| (1,1690) | 1:77:A:THR:HG21 | 1:80:A:VAL:HG13 | 15       | 0.11          |
| (1,1690) | 1:77:A:THR:HG21 | 1:80:A:VAL:HG21 | 15       | 0.11          |
| (1,1690) | 1:77:A:THR:HG21 | 1:80:A:VAL:HG22 | 15       | 0.11          |
| (1,1690) | 1:77:A:THR:HG21 | 1:80:A:VAL:HG23 | 15       | 0.11          |
| (1,1690) | 1:77:A:THR:HG22 | 1:80:A:VAL:HG11 | 15       | 0.11          |
| (1,1690) | 1:77:A:THR:HG22 | 1:80:A:VAL:HG12 | 15       | 0.11          |
| (1,1690) | 1:77:A:THR:HG22 | 1:80:A:VAL:HG13 | 15       | 0.11          |
| (1,1690) | 1:77:A:THR:HG22 | 1:80:A:VAL:HG21 | 15       | 0.11          |
| (1,1690) | 1:77:A:THR:HG22 | 1:80:A:VAL:HG22 | 15       | 0.11          |
| (1,1690) | 1:77:A:THR:HG22 | 1:80:A:VAL:HG23 | 15       | 0.11          |
| (1,1690) | 1:77:A:THR:HG23 | 1:80:A:VAL:HG11 | 15       | 0.11          |
| (1,1690) | 1:77:A:THR:HG23 | 1:80:A:VAL:HG12 | 15       | 0.11          |
| (1,1690) | 1:77:A:THR:HG23 | 1:80:A:VAL:HG13 | 15       | 0.11          |
| (1,1690) | 1:77:A:THR:HG23 | 1:80:A:VAL:HG21 | 15       | 0.11          |
| (1,1690) | 1:77:A:THR:HG23 | 1:80:A:VAL:HG22 | 15       | 0.11          |
| (1,1690) | 1:77:A:THR:HG23 | 1:80:A:VAL:HG23 | 15       | 0.11          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG11 | 3        | 0.11          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG12 | 3        | 0.11          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG13 | 3        | 0.11          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG21 | 3        | 0.11          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG22 | 3        | 0.11          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG23 | 3        | 0.11          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG11 | 11       | 0.11          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG12 | 11       | 0.11          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG13 | 11       | 0.11          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG21 | 11       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG22 | 11       | 0.11          |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG23 | 11       | 0.11          |
| (1,1680) | 1:77:A:THR:HG21 | 1:78:A:MET:HG2  | 1        | 0.11          |
| (1,1680) | 1:77:A:THR:HG21 | 1:78:A:MET:HG3  | 1        | 0.11          |
| (1,1680) | 1:77:A:THR:HG22 | 1:78:A:MET:HG2  | 1        | 0.11          |
| (1,1680) | 1:77:A:THR:HG22 | 1:78:A:MET:HG3  | 1        | 0.11          |
| (1,1680) | 1:77:A:THR:HG23 | 1:78:A:MET:HG2  | 1        | 0.11          |
| (1,1680) | 1:77:A:THR:HG23 | 1:78:A:MET:HG3  | 1        | 0.11          |
| (1,1680) | 1:77:A:THR:HG21 | 1:78:A:MET:HG2  | 3        | 0.11          |
| (1,1680) | 1:77:A:THR:HG21 | 1:78:A:MET:HG3  | 3        | 0.11          |
| (1,1680) | 1:77:A:THR:HG22 | 1:78:A:MET:HG2  | 3        | 0.11          |
| (1,1680) | 1:77:A:THR:HG22 | 1:78:A:MET:HG3  | 3        | 0.11          |
| (1,1680) | 1:77:A:THR:HG23 | 1:78:A:MET:HG2  | 3        | 0.11          |
| (1,1680) | 1:77:A:THR:HG23 | 1:78:A:MET:HG3  | 3        | 0.11          |
| (1,1680) | 1:77:A:THR:HG21 | 1:78:A:MET:HG2  | 5        | 0.11          |
| (1,1680) | 1:77:A:THR:HG21 | 1:78:A:MET:HG3  | 5        | 0.11          |
| (1,1680) | 1:77:A:THR:HG22 | 1:78:A:MET:HG2  | 5        | 0.11          |
| (1,1680) | 1:77:A:THR:HG22 | 1:78:A:MET:HG3  | 5        | 0.11          |
| (1,1680) | 1:77:A:THR:HG23 | 1:78:A:MET:HG2  | 5        | 0.11          |
| (1,1680) | 1:77:A:THR:HG23 | 1:78:A:MET:HG3  | 5        | 0.11          |
| (1,1680) | 1:77:A:THR:HG21 | 1:78:A:MET:HG2  | 8        | 0.11          |
| (1,1680) | 1:77:A:THR:HG21 | 1:78:A:MET:HG3  | 8        | 0.11          |
| (1,1680) | 1:77:A:THR:HG22 | 1:78:A:MET:HG2  | 8        | 0.11          |
| (1,1680) | 1:77:A:THR:HG22 | 1:78:A:MET:HG3  | 8        | 0.11          |
| (1,1680) | 1:77:A:THR:HG23 | 1:78:A:MET:HG2  | 8        | 0.11          |
| (1,1680) | 1:77:A:THR:HG23 | 1:78:A:MET:HG3  | 8        | 0.11          |
| (1,1669) | 1:76:A:LEU:HD11 | 1:80:A:VAL:HB   | 17       | 0.11          |
| (1,1669) | 1:76:A:LEU:HD12 | 1:80:A:VAL:HB   | 17       | 0.11          |
| (1,1669) | 1:76:A:LEU:HD13 | 1:80:A:VAL:HB   | 17       | 0.11          |
| (1,1669) | 1:76:A:LEU:HD21 | 1:80:A:VAL:HB   | 17       | 0.11          |
| (1,1669) | 1:76:A:LEU:HD22 | 1:80:A:VAL:HB   | 17       | 0.11          |
| (1,1669) | 1:76:A:LEU:HD23 | 1:80:A:VAL:HB   | 17       | 0.11          |
| (1,1635) | 1:75:A:LEU:HA   | 1:75:A:LEU:HG   | 19       | 0.11          |
| (1,1608) | 1:73:A:PRO:HA   | 1:73:A:PRO:HD2  | 9        | 0.11          |
| (1,1608) | 1:73:A:PRO:HA   | 1:73:A:PRO:HD3  | 9        | 0.11          |
| (1,1608) | 1:73:A:PRO:HA   | 1:73:A:PRO:HD2  | 19       | 0.11          |
| (1,1608) | 1:73:A:PRO:HA   | 1:73:A:PRO:HD3  | 19       | 0.11          |
| (1,1597) | 1:72:A:ARG:HG2  | 1:74:A:ASP:H    | 17       | 0.11          |
| (1,1597) | 1:72:A:ARG:HG3  | 1:74:A:ASP:H    | 17       | 0.11          |
| (1,1547) | 1:69:A:ILE:HB   | 1:69:A:ILE:H    | 17       | 0.11          |
| (1,1541) | 1:68:A:GLU:HG2  | 1:76:A:LEU:HD11 | 9        | 0.11          |
| (1,1541) | 1:68:A:GLU:HG2  | 1:76:A:LEU:HD12 | 9        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1541) | 1:68:A:GLU:HG2  | 1:76:A:LEU:HD13 | 9        | 0.11          |
| (1,1541) | 1:68:A:GLU:HG2  | 1:76:A:LEU:HD21 | 9        | 0.11          |
| (1,1541) | 1:68:A:GLU:HG2  | 1:76:A:LEU:HD22 | 9        | 0.11          |
| (1,1541) | 1:68:A:GLU:HG2  | 1:76:A:LEU:HD23 | 9        | 0.11          |
| (1,1541) | 1:68:A:GLU:HG3  | 1:76:A:LEU:HD11 | 9        | 0.11          |
| (1,1541) | 1:68:A:GLU:HG3  | 1:76:A:LEU:HD12 | 9        | 0.11          |
| (1,1541) | 1:68:A:GLU:HG3  | 1:76:A:LEU:HD13 | 9        | 0.11          |
| (1,1541) | 1:68:A:GLU:HG3  | 1:76:A:LEU:HD21 | 9        | 0.11          |
| (1,1541) | 1:68:A:GLU:HG3  | 1:76:A:LEU:HD22 | 9        | 0.11          |
| (1,1541) | 1:68:A:GLU:HG3  | 1:76:A:LEU:HD23 | 9        | 0.11          |
| (1,1538) | 1:68:A:GLU:HA   | 1:71:A:ARG:HD2  | 1        | 0.11          |
| (1,1538) | 1:68:A:GLU:HA   | 1:71:A:ARG:HD3  | 1        | 0.11          |
| (1,1538) | 1:68:A:GLU:HA   | 1:71:A:ARG:HD2  | 20       | 0.11          |
| (1,1538) | 1:68:A:GLU:HA   | 1:71:A:ARG:HD3  | 20       | 0.11          |
| (1,1517) | 1:67:A:PHE:HD1  | 1:76:A:LEU:HG   | 10       | 0.11          |
| (1,1517) | 1:67:A:PHE:HD2  | 1:76:A:LEU:HG   | 10       | 0.11          |
| (1,1516) | 1:67:A:PHE:H    | 1:76:A:LEU:HG   | 17       | 0.11          |
| (1,1507) | 1:67:A:PHE:HE1  | 1:76:A:LEU:HB2  | 6        | 0.11          |
| (1,1507) | 1:67:A:PHE:HE1  | 1:76:A:LEU:HB3  | 6        | 0.11          |
| (1,1507) | 1:67:A:PHE:HE2  | 1:76:A:LEU:HB2  | 6        | 0.11          |
| (1,1507) | 1:67:A:PHE:HE2  | 1:76:A:LEU:HB3  | 6        | 0.11          |
| (1,1461) | 1:66:A:ILE:HG21 | 1:67:A:PHE:HA   | 13       | 0.11          |
| (1,1461) | 1:66:A:ILE:HG22 | 1:67:A:PHE:HA   | 13       | 0.11          |
| (1,1461) | 1:66:A:ILE:HG23 | 1:67:A:PHE:HA   | 13       | 0.11          |
| (1,1452) | 1:66:A:ILE:HA   | 1:66:A:ILE:HG12 | 12       | 0.11          |
| (1,1452) | 1:66:A:ILE:HA   | 1:66:A:ILE:HG13 | 12       | 0.11          |
| (1,1445) | 1:66:A:ILE:HG12 | 1:66:A:ILE:H    | 12       | 0.11          |
| (1,1445) | 1:66:A:ILE:HG13 | 1:66:A:ILE:H    | 12       | 0.11          |
| (1,1445) | 1:66:A:ILE:HG12 | 1:66:A:ILE:H    | 14       | 0.11          |
| (1,1445) | 1:66:A:ILE:HG13 | 1:66:A:ILE:H    | 14       | 0.11          |
| (1,1445) | 1:66:A:ILE:HG12 | 1:66:A:ILE:H    | 15       | 0.11          |
| (1,1445) | 1:66:A:ILE:HG13 | 1:66:A:ILE:H    | 15       | 0.11          |
| (1,1445) | 1:66:A:ILE:HG12 | 1:66:A:ILE:H    | 17       | 0.11          |
| (1,1445) | 1:66:A:ILE:HG13 | 1:66:A:ILE:H    | 17       | 0.11          |
| (1,1445) | 1:66:A:ILE:HG12 | 1:66:A:ILE:H    | 18       | 0.11          |
| (1,1445) | 1:66:A:ILE:HG13 | 1:66:A:ILE:H    | 18       | 0.11          |
| (1,1439) | 1:65:A:HIS:HA   | 1:69:A:ILE:H    | 9        | 0.11          |
| (1,1437) | 1:65:A:HIS:HA   | 1:68:A:GLU:H    | 11       | 0.11          |
| (1,1434) | 1:65:A:HIS:HB2  | 1:67:A:PHE:HD1  | 2        | 0.11          |
| (1,1434) | 1:65:A:HIS:HB2  | 1:67:A:PHE:HD2  | 2        | 0.11          |
| (1,1434) | 1:65:A:HIS:HB3  | 1:67:A:PHE:HD1  | 2        | 0.11          |
| (1,1434) | 1:65:A:HIS:HB3  | 1:67:A:PHE:HD2  | 2        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1428) | 1:65:A:HIS:HD2  | 1:66:A:ILE:HG12 | 3        | 0.11          |
| (1,1428) | 1:65:A:HIS:HD2  | 1:66:A:ILE:HG13 | 3        | 0.11          |
| (1,1426) | 1:65:A:HIS:H    | 1:66:A:ILE:HB   | 5        | 0.11          |
| (1,1399) | 1:64:A:GLU:HA   | 1:67:A:PHE:H    | 2        | 0.11          |
| (1,1399) | 1:64:A:GLU:HA   | 1:67:A:PHE:H    | 19       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG11 | 10       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG12 | 10       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG13 | 10       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG21 | 10       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG22 | 10       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG23 | 10       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG11 | 10       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG12 | 10       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG13 | 10       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG21 | 10       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG22 | 10       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG23 | 10       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG11 | 10       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG12 | 10       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG13 | 10       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG21 | 10       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG22 | 10       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG23 | 10       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG11 | 18       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG12 | 18       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG13 | 18       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG21 | 18       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG22 | 18       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG21 | 1:79:A:VAL:HG23 | 18       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG11 | 18       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG12 | 18       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG13 | 18       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG21 | 18       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG22 | 18       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG22 | 1:79:A:VAL:HG23 | 18       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG11 | 18       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG12 | 18       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG13 | 18       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG21 | 18       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG22 | 18       | 0.11          |
| (1,1388) | 1:63:A:ILE:HG23 | 1:79:A:VAL:HG23 | 18       | 0.11          |
| (1,1379) | 1:63:A:ILE:HD11 | 1:67:A:PHE:H    | 2        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1379) | 1:63:A:ILE:HD12 | 1:67:A:PHE:H    | 2        | 0.11          |
| (1,1379) | 1:63:A:ILE:HD13 | 1:67:A:PHE:H    | 2        | 0.11          |
| (1,1368) | 1:63:A:ILE:HB   | 1:66:A:ILE:HD11 | 17       | 0.11          |
| (1,1368) | 1:63:A:ILE:HB   | 1:66:A:ILE:HD12 | 17       | 0.11          |
| (1,1368) | 1:63:A:ILE:HB   | 1:66:A:ILE:HD13 | 17       | 0.11          |
| (1,1349) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HD11 | 12       | 0.11          |
| (1,1349) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HD12 | 12       | 0.11          |
| (1,1349) | 1:62:A:TYR:HE1  | 1:66:A:ILE:HD13 | 12       | 0.11          |
| (1,1349) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HD11 | 12       | 0.11          |
| (1,1349) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HD12 | 12       | 0.11          |
| (1,1349) | 1:62:A:TYR:HE2  | 1:66:A:ILE:HD13 | 12       | 0.11          |
| (1,1324) | 1:61:A:SER:H    | 1:65:A:HIS:H    | 15       | 0.11          |
| (1,1319) | 1:61:A:SER:HA   | 1:63:A:ILE:HG21 | 5        | 0.11          |
| (1,1319) | 1:61:A:SER:HA   | 1:63:A:ILE:HG22 | 5        | 0.11          |
| (1,1319) | 1:61:A:SER:HA   | 1:63:A:ILE:HG23 | 5        | 0.11          |
| (1,1319) | 1:61:A:SER:HA   | 1:63:A:ILE:HG21 | 13       | 0.11          |
| (1,1319) | 1:61:A:SER:HA   | 1:63:A:ILE:HG22 | 13       | 0.11          |
| (1,1319) | 1:61:A:SER:HA   | 1:63:A:ILE:HG23 | 13       | 0.11          |
| (1,1319) | 1:61:A:SER:HA   | 1:63:A:ILE:HG21 | 19       | 0.11          |
| (1,1319) | 1:61:A:SER:HA   | 1:63:A:ILE:HG22 | 19       | 0.11          |
| (1,1319) | 1:61:A:SER:HA   | 1:63:A:ILE:HG23 | 19       | 0.11          |
| (1,1304) | 1:60:A:LEU:HD11 | 1:64:A:GLU:HG2  | 13       | 0.11          |
| (1,1304) | 1:60:A:LEU:HD11 | 1:64:A:GLU:HG3  | 13       | 0.11          |
| (1,1304) | 1:60:A:LEU:HD12 | 1:64:A:GLU:HG2  | 13       | 0.11          |
| (1,1304) | 1:60:A:LEU:HD12 | 1:64:A:GLU:HG3  | 13       | 0.11          |
| (1,1304) | 1:60:A:LEU:HD13 | 1:64:A:GLU:HG2  | 13       | 0.11          |
| (1,1304) | 1:60:A:LEU:HD13 | 1:64:A:GLU:HG3  | 13       | 0.11          |
| (1,1304) | 1:60:A:LEU:HD21 | 1:64:A:GLU:HG2  | 13       | 0.11          |
| (1,1304) | 1:60:A:LEU:HD21 | 1:64:A:GLU:HG3  | 13       | 0.11          |
| (1,1304) | 1:60:A:LEU:HD22 | 1:64:A:GLU:HG2  | 13       | 0.11          |
| (1,1304) | 1:60:A:LEU:HD22 | 1:64:A:GLU:HG3  | 13       | 0.11          |
| (1,1304) | 1:60:A:LEU:HD23 | 1:64:A:GLU:HG2  | 13       | 0.11          |
| (1,1304) | 1:60:A:LEU:HD23 | 1:64:A:GLU:HG3  | 13       | 0.11          |
| (1,1292) | 1:60:A:LEU:HA   | 1:60:A:LEU:HD11 | 4        | 0.11          |
| (1,1292) | 1:60:A:LEU:HA   | 1:60:A:LEU:HD12 | 4        | 0.11          |
| (1,1292) | 1:60:A:LEU:HA   | 1:60:A:LEU:HD13 | 4        | 0.11          |
| (1,1292) | 1:60:A:LEU:HA   | 1:60:A:LEU:HD21 | 4        | 0.11          |
| (1,1292) | 1:60:A:LEU:HA   | 1:60:A:LEU:HD22 | 4        | 0.11          |
| (1,1292) | 1:60:A:LEU:HA   | 1:60:A:LEU:HD23 | 4        | 0.11          |
| (1,1292) | 1:60:A:LEU:HA   | 1:60:A:LEU:HD11 | 6        | 0.11          |
| (1,1292) | 1:60:A:LEU:HA   | 1:60:A:LEU:HD12 | 6        | 0.11          |
| (1,1292) | 1:60:A:LEU:HA   | 1:60:A:LEU:HD13 | 6        | 0.11          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD21 | 6        | 0.11          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD22 | 6        | 0.11          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD23 | 6        | 0.11          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD11 | 8        | 0.11          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD12 | 8        | 0.11          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD13 | 8        | 0.11          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD21 | 8        | 0.11          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD22 | 8        | 0.11          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD23 | 8        | 0.11          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD11 | 11       | 0.11          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD12 | 11       | 0.11          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD13 | 11       | 0.11          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD21 | 11       | 0.11          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD22 | 11       | 0.11          |
| (1,1292) | 1:60:A:LEU:HA  | 1:60:A:LEU:HD23 | 11       | 0.11          |
| (1,1288) | 1:59:A:ASN:HA  | 1:60:A:LEU:HD11 | 8        | 0.11          |
| (1,1288) | 1:59:A:ASN:HA  | 1:60:A:LEU:HD12 | 8        | 0.11          |
| (1,1288) | 1:59:A:ASN:HA  | 1:60:A:LEU:HD13 | 8        | 0.11          |
| (1,1288) | 1:59:A:ASN:HA  | 1:60:A:LEU:HD21 | 8        | 0.11          |
| (1,1288) | 1:59:A:ASN:HA  | 1:60:A:LEU:HD22 | 8        | 0.11          |
| (1,1288) | 1:59:A:ASN:HA  | 1:60:A:LEU:HD23 | 8        | 0.11          |
| (1,1277) | 1:58:A:ASP:H   | 1:60:A:LEU:H    | 3        | 0.11          |
| (1,1277) | 1:58:A:ASP:H   | 1:60:A:LEU:H    | 13       | 0.11          |
| (1,1274) | 1:58:A:ASP:H   | 1:59:A:ASN:HD21 | 17       | 0.11          |
| (1,1274) | 1:58:A:ASP:H   | 1:59:A:ASN:HD22 | 17       | 0.11          |
| (1,1267) | 1:57:A:LYS:HD2 | 1:59:A:ASN:H    | 3        | 0.11          |
| (1,1267) | 1:57:A:LYS:HD3 | 1:59:A:ASN:H    | 3        | 0.11          |
| (1,1259) | 1:57:A:LYS:HE2 | 1:58:A:ASP:H    | 4        | 0.11          |
| (1,1259) | 1:57:A:LYS:HE3 | 1:58:A:ASP:H    | 4        | 0.11          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD2  | 1        | 0.11          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD3  | 1        | 0.11          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD2  | 2        | 0.11          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD3  | 2        | 0.11          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD2  | 11       | 0.11          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD3  | 11       | 0.11          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD2  | 20       | 0.11          |
| (1,1256) | 1:57:A:LYS:HA  | 1:57:A:LYS:HD3  | 20       | 0.11          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG2  | 8        | 0.11          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG3  | 8        | 0.11          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG2  | 17       | 0.11          |
| (1,1255) | 1:57:A:LYS:HA  | 1:57:A:LYS:HG3  | 17       | 0.11          |
| (1,1252) | 1:56:A:ASP:HB2 | 1:59:A:ASN:HD21 | 7        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1252) | 1:56:A:ASP:HB2  | 1:59:A:ASN:HD22 | 7        | 0.11          |
| (1,1252) | 1:56:A:ASP:HB3  | 1:59:A:ASN:HD21 | 7        | 0.11          |
| (1,1252) | 1:56:A:ASP:HB3  | 1:59:A:ASN:HD22 | 7        | 0.11          |
| (1,1241) | 1:56:A:ASP:HB2  | 1:57:A:LYS:H    | 19       | 0.11          |
| (1,1241) | 1:56:A:ASP:HB3  | 1:57:A:LYS:H    | 19       | 0.11          |
| (1,1233) | 1:55:A:LEU:HG   | 1:63:A:ILE:HB   | 12       | 0.11          |
| (1,1233) | 1:55:A:LEU:HG   | 1:63:A:ILE:HB   | 15       | 0.11          |
| (1,1233) | 1:55:A:LEU:HG   | 1:63:A:ILE:HB   | 17       | 0.11          |
| (1,1233) | 1:55:A:LEU:HG   | 1:63:A:ILE:HB   | 18       | 0.11          |
| (1,1228) | 1:55:A:LEU:HG   | 1:59:A:ASN:HD21 | 14       | 0.11          |
| (1,1228) | 1:55:A:LEU:HG   | 1:59:A:ASN:HD22 | 14       | 0.11          |
| (1,1228) | 1:55:A:LEU:HG   | 1:59:A:ASN:HD21 | 16       | 0.11          |
| (1,1228) | 1:55:A:LEU:HG   | 1:59:A:ASN:HD22 | 16       | 0.11          |
| (1,1223) | 1:55:A:LEU:HG   | 1:56:A:ASP:HA   | 1        | 0.11          |
| (1,1223) | 1:55:A:LEU:HG   | 1:56:A:ASP:HA   | 2        | 0.11          |
| (1,1223) | 1:55:A:LEU:HG   | 1:56:A:ASP:HA   | 12       | 0.11          |
| (1,1212) | 1:54:A:LYS:HE2  | 1:62:A:TYR:HD1  | 3        | 0.11          |
| (1,1212) | 1:54:A:LYS:HE2  | 1:62:A:TYR:HD2  | 3        | 0.11          |
| (1,1212) | 1:54:A:LYS:HE3  | 1:62:A:TYR:HD1  | 3        | 0.11          |
| (1,1212) | 1:54:A:LYS:HE3  | 1:62:A:TYR:HD2  | 3        | 0.11          |
| (1,1207) | 1:54:A:LYS:HG2  | 1:62:A:TYR:HE1  | 6        | 0.11          |
| (1,1207) | 1:54:A:LYS:HG2  | 1:62:A:TYR:HE2  | 6        | 0.11          |
| (1,1207) | 1:54:A:LYS:HG3  | 1:62:A:TYR:HE1  | 6        | 0.11          |
| (1,1207) | 1:54:A:LYS:HG3  | 1:62:A:TYR:HE2  | 6        | 0.11          |
| (1,1207) | 1:54:A:LYS:HG2  | 1:62:A:TYR:HE1  | 14       | 0.11          |
| (1,1207) | 1:54:A:LYS:HG2  | 1:62:A:TYR:HE2  | 14       | 0.11          |
| (1,1207) | 1:54:A:LYS:HG3  | 1:62:A:TYR:HE1  | 14       | 0.11          |
| (1,1207) | 1:54:A:LYS:HG3  | 1:62:A:TYR:HE2  | 14       | 0.11          |
| (1,1206) | 1:54:A:LYS:HB2  | 1:62:A:TYR:HE1  | 15       | 0.11          |
| (1,1206) | 1:54:A:LYS:HB2  | 1:62:A:TYR:HE2  | 15       | 0.11          |
| (1,1206) | 1:54:A:LYS:HB3  | 1:62:A:TYR:HE1  | 15       | 0.11          |
| (1,1206) | 1:54:A:LYS:HB3  | 1:62:A:TYR:HE2  | 15       | 0.11          |
| (1,1129) | 1:49:A:LEU:HG   | 1:62:A:TYR:HD1  | 16       | 0.11          |
| (1,1129) | 1:49:A:LEU:HG   | 1:62:A:TYR:HD2  | 16       | 0.11          |
| (1,1128) | 1:49:A:LEU:HD11 | 1:62:A:TYR:HE1  | 18       | 0.11          |
| (1,1128) | 1:49:A:LEU:HD11 | 1:62:A:TYR:HE2  | 18       | 0.11          |
| (1,1128) | 1:49:A:LEU:HD12 | 1:62:A:TYR:HE1  | 18       | 0.11          |
| (1,1128) | 1:49:A:LEU:HD12 | 1:62:A:TYR:HE2  | 18       | 0.11          |
| (1,1128) | 1:49:A:LEU:HD13 | 1:62:A:TYR:HE1  | 18       | 0.11          |
| (1,1128) | 1:49:A:LEU:HD13 | 1:62:A:TYR:HE2  | 18       | 0.11          |
| (1,1128) | 1:49:A:LEU:HD21 | 1:62:A:TYR:HE1  | 18       | 0.11          |
| (1,1128) | 1:49:A:LEU:HD21 | 1:62:A:TYR:HE2  | 18       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1128) | 1:49:A:LEU:HD22 | 1:62:A:TYR:HE1  | 18       | 0.11          |
| (1,1128) | 1:49:A:LEU:HD22 | 1:62:A:TYR:HE2  | 18       | 0.11          |
| (1,1128) | 1:49:A:LEU:HD23 | 1:62:A:TYR:HE1  | 18       | 0.11          |
| (1,1128) | 1:49:A:LEU:HD23 | 1:62:A:TYR:HE2  | 18       | 0.11          |
| (1,1105) | 1:49:A:LEU:HB2  | 1:52:A:HIS:HD2  | 2        | 0.11          |
| (1,1105) | 1:49:A:LEU:HB3  | 1:52:A:HIS:HD2  | 2        | 0.11          |
| (1,1018) | 1:46:A:PHE:HD1  | 1:46:A:PHE:H    | 6        | 0.11          |
| (1,1018) | 1:46:A:PHE:HD2  | 1:46:A:PHE:H    | 6        | 0.11          |
| (1,1010) | 1:45:A:TRP:HE1  | 1:66:A:ILE:HG12 | 13       | 0.11          |
| (1,1010) | 1:45:A:TRP:HE1  | 1:66:A:ILE:HG13 | 13       | 0.11          |
| (1,997)  | 1:45:A:TRP:HA   | 1:50:A:GLU:H    | 1        | 0.11          |
| (1,997)  | 1:45:A:TRP:HA   | 1:50:A:GLU:H    | 18       | 0.11          |
| (1,982)  | 1:45:A:TRP:HE1  | 1:46:A:PHE:HA   | 3        | 0.11          |
| (1,982)  | 1:45:A:TRP:HE1  | 1:46:A:PHE:HA   | 5        | 0.11          |
| (1,982)  | 1:45:A:TRP:HE1  | 1:46:A:PHE:HA   | 14       | 0.11          |
| (1,982)  | 1:45:A:TRP:HE1  | 1:46:A:PHE:HA   | 18       | 0.11          |
| (1,926)  | 1:41:A:THR:HB   | 1:42:A:GLY:H    | 2        | 0.11          |
| (1,926)  | 1:41:A:THR:HB   | 1:42:A:GLY:H    | 8        | 0.11          |
| (1,923)  | 1:41:A:THR:HB   | 1:41:A:THR:H    | 1        | 0.11          |
| (1,923)  | 1:41:A:THR:HB   | 1:41:A:THR:H    | 3        | 0.11          |
| (1,923)  | 1:41:A:THR:HB   | 1:41:A:THR:H    | 17       | 0.11          |
| (1,918)  | 1:40:A:THR:HA   | 1:41:A:THR:H    | 19       | 0.11          |
| (1,909)  | 1:39:A:ILE:HG12 | 1:48:A:PHE:H    | 2        | 0.11          |
| (1,909)  | 1:39:A:ILE:HG13 | 1:48:A:PHE:H    | 2        | 0.11          |
| (1,909)  | 1:39:A:ILE:HG12 | 1:48:A:PHE:H    | 20       | 0.11          |
| (1,909)  | 1:39:A:ILE:HG13 | 1:48:A:PHE:H    | 20       | 0.11          |
| (1,901)  | 1:39:A:ILE:HG12 | 1:45:A:TRP:HD1  | 8        | 0.11          |
| (1,901)  | 1:39:A:ILE:HG13 | 1:45:A:TRP:HD1  | 8        | 0.11          |
| (1,839)  | 1:36:A:SER:HB2  | 1:39:A:ILE:HD11 | 20       | 0.11          |
| (1,839)  | 1:36:A:SER:HB2  | 1:39:A:ILE:HD12 | 20       | 0.11          |
| (1,839)  | 1:36:A:SER:HB2  | 1:39:A:ILE:HD13 | 20       | 0.11          |
| (1,839)  | 1:36:A:SER:HB3  | 1:39:A:ILE:HD11 | 20       | 0.11          |
| (1,839)  | 1:36:A:SER:HB3  | 1:39:A:ILE:HD12 | 20       | 0.11          |
| (1,839)  | 1:36:A:SER:HB3  | 1:39:A:ILE:HD13 | 20       | 0.11          |
| (1,803)  | 1:35:A:LYS:HA   | 1:35:A:LYS:HG2  | 3        | 0.11          |
| (1,803)  | 1:35:A:LYS:HA   | 1:35:A:LYS:HG3  | 3        | 0.11          |
| (1,802)  | 1:35:A:LYS:HA   | 1:35:A:LYS:HD2  | 7        | 0.11          |
| (1,802)  | 1:35:A:LYS:HA   | 1:35:A:LYS:HD3  | 7        | 0.11          |
| (1,783)  | 1:32:A:PRO:HD2  | 1:35:A:LYS:HG2  | 1        | 0.11          |
| (1,783)  | 1:32:A:PRO:HD2  | 1:35:A:LYS:HG3  | 1        | 0.11          |
| (1,783)  | 1:32:A:PRO:HD3  | 1:35:A:LYS:HG2  | 1        | 0.11          |
| (1,783)  | 1:32:A:PRO:HD3  | 1:35:A:LYS:HG3  | 1        | 0.11          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,783) | 1:32:A:PRO:HD2  | 1:35:A:LYS:HG2 | 12       | 0.11          |
| (1,783) | 1:32:A:PRO:HD2  | 1:35:A:LYS:HG3 | 12       | 0.11          |
| (1,783) | 1:32:A:PRO:HD3  | 1:35:A:LYS:HG2 | 12       | 0.11          |
| (1,783) | 1:32:A:PRO:HD3  | 1:35:A:LYS:HG3 | 12       | 0.11          |
| (1,775) | 1:32:A:PRO:HA   | 1:32:A:PRO:HG2 | 1        | 0.11          |
| (1,775) | 1:32:A:PRO:HA   | 1:32:A:PRO:HG3 | 1        | 0.11          |
| (1,775) | 1:32:A:PRO:HA   | 1:32:A:PRO:HG2 | 12       | 0.11          |
| (1,775) | 1:32:A:PRO:HA   | 1:32:A:PRO:HG3 | 12       | 0.11          |
| (1,761) | 1:31:A:ILE:HD11 | 1:45:A:TRP:HD1 | 1        | 0.11          |
| (1,761) | 1:31:A:ILE:HD12 | 1:45:A:TRP:HD1 | 1        | 0.11          |
| (1,761) | 1:31:A:ILE:HD13 | 1:45:A:TRP:HD1 | 1        | 0.11          |
| (1,761) | 1:31:A:ILE:HD11 | 1:45:A:TRP:HD1 | 2        | 0.11          |
| (1,761) | 1:31:A:ILE:HD12 | 1:45:A:TRP:HD1 | 2        | 0.11          |
| (1,761) | 1:31:A:ILE:HD13 | 1:45:A:TRP:HD1 | 2        | 0.11          |
| (1,761) | 1:31:A:ILE:HD11 | 1:45:A:TRP:HD1 | 8        | 0.11          |
| (1,761) | 1:31:A:ILE:HD12 | 1:45:A:TRP:HD1 | 8        | 0.11          |
| (1,761) | 1:31:A:ILE:HD13 | 1:45:A:TRP:HD1 | 8        | 0.11          |
| (1,761) | 1:31:A:ILE:HD11 | 1:45:A:TRP:HD1 | 10       | 0.11          |
| (1,761) | 1:31:A:ILE:HD12 | 1:45:A:TRP:HD1 | 10       | 0.11          |
| (1,761) | 1:31:A:ILE:HD13 | 1:45:A:TRP:HD1 | 10       | 0.11          |
| (1,761) | 1:31:A:ILE:HD11 | 1:45:A:TRP:HD1 | 17       | 0.11          |
| (1,761) | 1:31:A:ILE:HD12 | 1:45:A:TRP:HD1 | 17       | 0.11          |
| (1,761) | 1:31:A:ILE:HD13 | 1:45:A:TRP:HD1 | 17       | 0.11          |
| (1,761) | 1:31:A:ILE:HD11 | 1:45:A:TRP:HD1 | 20       | 0.11          |
| (1,761) | 1:31:A:ILE:HD12 | 1:45:A:TRP:HD1 | 20       | 0.11          |
| (1,761) | 1:31:A:ILE:HD13 | 1:45:A:TRP:HD1 | 20       | 0.11          |
| (1,760) | 1:31:A:ILE:H    | 1:45:A:TRP:HZ2 | 1        | 0.11          |
| (1,743) | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD2 | 5        | 0.11          |
| (1,743) | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD3 | 5        | 0.11          |
| (1,743) | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD2 | 5        | 0.11          |
| (1,743) | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD3 | 5        | 0.11          |
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD2 | 5        | 0.11          |
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD3 | 5        | 0.11          |
| (1,743) | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD2 | 12       | 0.11          |
| (1,743) | 1:31:A:ILE:HD11 | 1:35:A:LYS:HD3 | 12       | 0.11          |
| (1,743) | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD2 | 12       | 0.11          |
| (1,743) | 1:31:A:ILE:HD12 | 1:35:A:LYS:HD3 | 12       | 0.11          |
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD2 | 12       | 0.11          |
| (1,743) | 1:31:A:ILE:HD13 | 1:35:A:LYS:HD3 | 12       | 0.11          |
| (1,736) | 1:31:A:ILE:HB   | 1:32:A:PRO:HA  | 10       | 0.11          |
| (1,736) | 1:31:A:ILE:HB   | 1:32:A:PRO:HA  | 11       | 0.11          |
| (1,736) | 1:31:A:ILE:HB   | 1:32:A:PRO:HA  | 13       | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,736) | 1:31:A:ILE:HB   | 1:32:A:PRO:HA   | 18       | 0.11          |
| (1,732) | 1:31:A:ILE:HD11 | 1:32:A:PRO:HA   | 10       | 0.11          |
| (1,732) | 1:31:A:ILE:HD12 | 1:32:A:PRO:HA   | 10       | 0.11          |
| (1,732) | 1:31:A:ILE:HD13 | 1:32:A:PRO:HA   | 10       | 0.11          |
| (1,724) | 1:31:A:ILE:HD11 | 1:31:A:ILE:H    | 14       | 0.11          |
| (1,724) | 1:31:A:ILE:HD12 | 1:31:A:ILE:H    | 14       | 0.11          |
| (1,724) | 1:31:A:ILE:HD13 | 1:31:A:ILE:H    | 14       | 0.11          |
| (1,724) | 1:31:A:ILE:HD11 | 1:31:A:ILE:H    | 20       | 0.11          |
| (1,724) | 1:31:A:ILE:HD12 | 1:31:A:ILE:H    | 20       | 0.11          |
| (1,724) | 1:31:A:ILE:HD13 | 1:31:A:ILE:H    | 20       | 0.11          |
| (1,713) | 1:29:A:GLU:HB2  | 1:31:A:ILE:H    | 5        | 0.11          |
| (1,713) | 1:29:A:GLU:HB3  | 1:31:A:ILE:H    | 5        | 0.11          |
| (1,675) | 1:27:A:CYS:H    | 1:31:A:ILE:HB   | 8        | 0.11          |
| (1,669) | 1:27:A:CYS:HB2  | 1:30:A:ASP:H    | 1        | 0.11          |
| (1,669) | 1:27:A:CYS:HB3  | 1:30:A:ASP:H    | 1        | 0.11          |
| (1,669) | 1:27:A:CYS:HB2  | 1:30:A:ASP:H    | 5        | 0.11          |
| (1,669) | 1:27:A:CYS:HB3  | 1:30:A:ASP:H    | 5        | 0.11          |
| (1,669) | 1:27:A:CYS:HB2  | 1:30:A:ASP:H    | 10       | 0.11          |
| (1,669) | 1:27:A:CYS:HB3  | 1:30:A:ASP:H    | 10       | 0.11          |
| (1,669) | 1:27:A:CYS:HB2  | 1:30:A:ASP:H    | 17       | 0.11          |
| (1,669) | 1:27:A:CYS:HB3  | 1:30:A:ASP:H    | 17       | 0.11          |
| (1,669) | 1:27:A:CYS:HB2  | 1:30:A:ASP:H    | 20       | 0.11          |
| (1,669) | 1:27:A:CYS:HB3  | 1:30:A:ASP:H    | 20       | 0.11          |
| (1,654) | 1:26:A:ALA:HB1  | 1:66:A:ILE:HA   | 12       | 0.11          |
| (1,654) | 1:26:A:ALA:HB2  | 1:66:A:ILE:HA   | 12       | 0.11          |
| (1,654) | 1:26:A:ALA:HB3  | 1:66:A:ILE:HA   | 12       | 0.11          |
| (1,643) | 1:26:A:ALA:HA   | 1:28:A:LYS:HB2  | 17       | 0.11          |
| (1,643) | 1:26:A:ALA:HA   | 1:28:A:LYS:HB3  | 17       | 0.11          |
| (1,643) | 1:26:A:ALA:HA   | 1:28:A:LYS:HB2  | 20       | 0.11          |
| (1,643) | 1:26:A:ALA:HA   | 1:28:A:LYS:HB3  | 20       | 0.11          |
| (1,626) | 1:24:A:LYS:HA   | 1:45:A:TRP:HE1  | 3        | 0.11          |
| (1,621) | 1:24:A:LYS:HB2  | 1:31:A:ILE:HG21 | 20       | 0.11          |
| (1,621) | 1:24:A:LYS:HB2  | 1:31:A:ILE:HG22 | 20       | 0.11          |
| (1,621) | 1:24:A:LYS:HB2  | 1:31:A:ILE:HG23 | 20       | 0.11          |
| (1,621) | 1:24:A:LYS:HB3  | 1:31:A:ILE:HG21 | 20       | 0.11          |
| (1,621) | 1:24:A:LYS:HB3  | 1:31:A:ILE:HG22 | 20       | 0.11          |
| (1,621) | 1:24:A:LYS:HB3  | 1:31:A:ILE:HG23 | 20       | 0.11          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG21 | 11       | 0.11          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG22 | 11       | 0.11          |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG23 | 11       | 0.11          |
| (1,566) | 1:22:A:GLN:HG2  | 1:25:A:SER:HB2  | 5        | 0.11          |
| (1,566) | 1:22:A:GLN:HG2  | 1:25:A:SER:HB3  | 5        | 0.11          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,566) | 1:22:A:GLN:HG3  | 1:25:A:SER:HB2 | 5        | 0.11          |
| (1,566) | 1:22:A:GLN:HG3  | 1:25:A:SER:HB3 | 5        | 0.11          |
| (1,566) | 1:22:A:GLN:HG2  | 1:25:A:SER:HB2 | 10       | 0.11          |
| (1,566) | 1:22:A:GLN:HG2  | 1:25:A:SER:HB3 | 10       | 0.11          |
| (1,566) | 1:22:A:GLN:HG3  | 1:25:A:SER:HB2 | 10       | 0.11          |
| (1,566) | 1:22:A:GLN:HG3  | 1:25:A:SER:HB3 | 10       | 0.11          |
| (1,555) | 1:22:A:GLN:HA   | 1:23:A:LEU:H   | 1        | 0.11          |
| (1,555) | 1:22:A:GLN:HA   | 1:23:A:LEU:H   | 3        | 0.11          |
| (1,537) | 1:21:A:GLU:HA   | 1:21:A:GLU:HG2 | 11       | 0.11          |
| (1,537) | 1:21:A:GLU:HA   | 1:21:A:GLU:HG3 | 11       | 0.11          |
| (1,534) | 1:20:A:LEU:HD11 | 1:67:A:PHE:HE1 | 3        | 0.11          |
| (1,534) | 1:20:A:LEU:HD11 | 1:67:A:PHE:HE2 | 3        | 0.11          |
| (1,534) | 1:20:A:LEU:HD12 | 1:67:A:PHE:HE1 | 3        | 0.11          |
| (1,534) | 1:20:A:LEU:HD12 | 1:67:A:PHE:HE2 | 3        | 0.11          |
| (1,534) | 1:20:A:LEU:HD13 | 1:67:A:PHE:HE1 | 3        | 0.11          |
| (1,534) | 1:20:A:LEU:HD13 | 1:67:A:PHE:HE2 | 3        | 0.11          |
| (1,534) | 1:20:A:LEU:HD21 | 1:67:A:PHE:HE1 | 3        | 0.11          |
| (1,534) | 1:20:A:LEU:HD21 | 1:67:A:PHE:HE2 | 3        | 0.11          |
| (1,534) | 1:20:A:LEU:HD22 | 1:67:A:PHE:HE1 | 3        | 0.11          |
| (1,534) | 1:20:A:LEU:HD22 | 1:67:A:PHE:HE2 | 3        | 0.11          |
| (1,534) | 1:20:A:LEU:HD23 | 1:67:A:PHE:HE1 | 3        | 0.11          |
| (1,534) | 1:20:A:LEU:HD23 | 1:67:A:PHE:HE2 | 3        | 0.11          |
| (1,534) | 1:20:A:LEU:HD11 | 1:67:A:PHE:HE1 | 10       | 0.11          |
| (1,534) | 1:20:A:LEU:HD11 | 1:67:A:PHE:HE2 | 10       | 0.11          |
| (1,534) | 1:20:A:LEU:HD12 | 1:67:A:PHE:HE1 | 10       | 0.11          |
| (1,534) | 1:20:A:LEU:HD12 | 1:67:A:PHE:HE2 | 10       | 0.11          |
| (1,534) | 1:20:A:LEU:HD13 | 1:67:A:PHE:HE1 | 10       | 0.11          |
| (1,534) | 1:20:A:LEU:HD13 | 1:67:A:PHE:HE2 | 10       | 0.11          |
| (1,534) | 1:20:A:LEU:HD21 | 1:67:A:PHE:HE1 | 10       | 0.11          |
| (1,534) | 1:20:A:LEU:HD21 | 1:67:A:PHE:HE2 | 10       | 0.11          |
| (1,534) | 1:20:A:LEU:HD22 | 1:67:A:PHE:HE1 | 10       | 0.11          |
| (1,534) | 1:20:A:LEU:HD22 | 1:67:A:PHE:HE2 | 10       | 0.11          |
| (1,534) | 1:20:A:LEU:HD23 | 1:67:A:PHE:HE1 | 10       | 0.11          |
| (1,534) | 1:20:A:LEU:HD23 | 1:67:A:PHE:HE2 | 10       | 0.11          |
| (1,534) | 1:20:A:LEU:HD11 | 1:67:A:PHE:HE1 | 16       | 0.11          |
| (1,534) | 1:20:A:LEU:HD11 | 1:67:A:PHE:HE2 | 16       | 0.11          |
| (1,534) | 1:20:A:LEU:HD12 | 1:67:A:PHE:HE1 | 16       | 0.11          |
| (1,534) | 1:20:A:LEU:HD12 | 1:67:A:PHE:HE2 | 16       | 0.11          |
| (1,534) | 1:20:A:LEU:HD13 | 1:67:A:PHE:HE1 | 16       | 0.11          |
| (1,534) | 1:20:A:LEU:HD13 | 1:67:A:PHE:HE2 | 16       | 0.11          |
| (1,534) | 1:20:A:LEU:HD21 | 1:67:A:PHE:HE1 | 16       | 0.11          |
| (1,534) | 1:20:A:LEU:HD21 | 1:67:A:PHE:HE2 | 16       | 0.11          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,534) | 1:20:A:LEU:HD22 | 1:67:A:PHE:HE1 | 16       | 0.11          |
| (1,534) | 1:20:A:LEU:HD22 | 1:67:A:PHE:HE2 | 16       | 0.11          |
| (1,534) | 1:20:A:LEU:HD23 | 1:67:A:PHE:HE1 | 16       | 0.11          |
| (1,534) | 1:20:A:LEU:HD23 | 1:67:A:PHE:HE2 | 16       | 0.11          |
| (1,534) | 1:20:A:LEU:HD11 | 1:67:A:PHE:HE1 | 17       | 0.11          |
| (1,534) | 1:20:A:LEU:HD11 | 1:67:A:PHE:HE2 | 17       | 0.11          |
| (1,534) | 1:20:A:LEU:HD12 | 1:67:A:PHE:HE1 | 17       | 0.11          |
| (1,534) | 1:20:A:LEU:HD12 | 1:67:A:PHE:HE2 | 17       | 0.11          |
| (1,534) | 1:20:A:LEU:HD13 | 1:67:A:PHE:HE1 | 17       | 0.11          |
| (1,534) | 1:20:A:LEU:HD13 | 1:67:A:PHE:HE2 | 17       | 0.11          |
| (1,534) | 1:20:A:LEU:HD21 | 1:67:A:PHE:HE1 | 17       | 0.11          |
| (1,534) | 1:20:A:LEU:HD21 | 1:67:A:PHE:HE2 | 17       | 0.11          |
| (1,534) | 1:20:A:LEU:HD22 | 1:67:A:PHE:HE1 | 17       | 0.11          |
| (1,534) | 1:20:A:LEU:HD22 | 1:67:A:PHE:HE2 | 17       | 0.11          |
| (1,534) | 1:20:A:LEU:HD23 | 1:67:A:PHE:HE1 | 17       | 0.11          |
| (1,534) | 1:20:A:LEU:HD23 | 1:67:A:PHE:HE2 | 17       | 0.11          |
| (1,490) | 1:20:A:LEU:HA   | 1:20:A:LEU:HG  | 5        | 0.11          |
| (1,490) | 1:20:A:LEU:HA   | 1:20:A:LEU:HG  | 7        | 0.11          |
| (1,487) | 1:20:A:LEU:HG   | 1:20:A:LEU:H   | 1        | 0.11          |
| (1,476) | 1:19:A:ASP:H    | 1:20:A:LEU:H   | 5        | 0.11          |
| (1,476) | 1:19:A:ASP:H    | 1:20:A:LEU:H   | 6        | 0.11          |
| (1,476) | 1:19:A:ASP:H    | 1:20:A:LEU:H   | 7        | 0.11          |
| (1,476) | 1:19:A:ASP:H    | 1:20:A:LEU:H   | 10       | 0.11          |
| (1,476) | 1:19:A:ASP:H    | 1:20:A:LEU:H   | 11       | 0.11          |
| (1,476) | 1:19:A:ASP:H    | 1:20:A:LEU:H   | 18       | 0.11          |
| (1,476) | 1:19:A:ASP:H    | 1:20:A:LEU:H   | 19       | 0.11          |
| (1,476) | 1:19:A:ASP:H    | 1:20:A:LEU:H   | 20       | 0.11          |
| (1,469) | 1:18:A:GLU:HA   | 1:20:A:LEU:HB2 | 17       | 0.11          |
| (1,469) | 1:18:A:GLU:HA   | 1:20:A:LEU:HB3 | 17       | 0.11          |
| (1,459) | 1:17:A:LEU:HG   | 1:40:A:THR:HB  | 6        | 0.11          |
| (1,425) | 1:16:A:THR:HG21 | 1:18:A:GLU:H   | 18       | 0.11          |
| (1,425) | 1:16:A:THR:HG22 | 1:18:A:GLU:H   | 18       | 0.11          |
| (1,425) | 1:16:A:THR:HG23 | 1:18:A:GLU:H   | 18       | 0.11          |
| (1,420) | 1:16:A:THR:HG21 | 1:17:A:LEU:H   | 1        | 0.11          |
| (1,420) | 1:16:A:THR:HG22 | 1:17:A:LEU:H   | 1        | 0.11          |
| (1,420) | 1:16:A:THR:HG23 | 1:17:A:LEU:H   | 1        | 0.11          |
| (1,420) | 1:16:A:THR:HG21 | 1:17:A:LEU:H   | 3        | 0.11          |
| (1,420) | 1:16:A:THR:HG22 | 1:17:A:LEU:H   | 3        | 0.11          |
| (1,420) | 1:16:A:THR:HG23 | 1:17:A:LEU:H   | 3        | 0.11          |
| (1,420) | 1:16:A:THR:HG21 | 1:17:A:LEU:H   | 8        | 0.11          |
| (1,420) | 1:16:A:THR:HG22 | 1:17:A:LEU:H   | 8        | 0.11          |
| (1,420) | 1:16:A:THR:HG23 | 1:17:A:LEU:H   | 8        | 0.11          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,420) | 1:16:A:THR:HG21 | 1:17:A:LEU:H   | 17       | 0.11          |
| (1,420) | 1:16:A:THR:HG22 | 1:17:A:LEU:H   | 17       | 0.11          |
| (1,420) | 1:16:A:THR:HG23 | 1:17:A:LEU:H   | 17       | 0.11          |
| (1,418) | 1:16:A:THR:HB   | 1:16:A:THR:H   | 17       | 0.11          |
| (1,415) | 1:15:A:ILE:HA   | 1:75:A:LEU:HG  | 9        | 0.11          |
| (1,405) | 1:15:A:ILE:HD11 | 1:43:A:SER:H   | 3        | 0.11          |
| (1,405) | 1:15:A:ILE:HD12 | 1:43:A:SER:H   | 3        | 0.11          |
| (1,405) | 1:15:A:ILE:HD13 | 1:43:A:SER:H   | 3        | 0.11          |
| (1,405) | 1:15:A:ILE:HD11 | 1:43:A:SER:H   | 7        | 0.11          |
| (1,405) | 1:15:A:ILE:HD12 | 1:43:A:SER:H   | 7        | 0.11          |
| (1,405) | 1:15:A:ILE:HD13 | 1:43:A:SER:H   | 7        | 0.11          |
| (1,405) | 1:15:A:ILE:HD11 | 1:43:A:SER:H   | 19       | 0.11          |
| (1,405) | 1:15:A:ILE:HD12 | 1:43:A:SER:H   | 19       | 0.11          |
| (1,405) | 1:15:A:ILE:HD13 | 1:43:A:SER:H   | 19       | 0.11          |
| (1,398) | 1:15:A:ILE:HD11 | 1:23:A:LEU:HB2 | 2        | 0.11          |
| (1,398) | 1:15:A:ILE:HD11 | 1:23:A:LEU:HB3 | 2        | 0.11          |
| (1,398) | 1:15:A:ILE:HD12 | 1:23:A:LEU:HB2 | 2        | 0.11          |
| (1,398) | 1:15:A:ILE:HD12 | 1:23:A:LEU:HB3 | 2        | 0.11          |
| (1,398) | 1:15:A:ILE:HD13 | 1:23:A:LEU:HB2 | 2        | 0.11          |
| (1,398) | 1:15:A:ILE:HD13 | 1:23:A:LEU:HB3 | 2        | 0.11          |
| (1,398) | 1:15:A:ILE:HD11 | 1:23:A:LEU:HB2 | 10       | 0.11          |
| (1,398) | 1:15:A:ILE:HD11 | 1:23:A:LEU:HB3 | 10       | 0.11          |
| (1,398) | 1:15:A:ILE:HD12 | 1:23:A:LEU:HB2 | 10       | 0.11          |
| (1,398) | 1:15:A:ILE:HD12 | 1:23:A:LEU:HB3 | 10       | 0.11          |
| (1,398) | 1:15:A:ILE:HD13 | 1:23:A:LEU:HB2 | 10       | 0.11          |
| (1,398) | 1:15:A:ILE:HD13 | 1:23:A:LEU:HB3 | 10       | 0.11          |
| (1,398) | 1:15:A:ILE:HD11 | 1:23:A:LEU:HB2 | 15       | 0.11          |
| (1,398) | 1:15:A:ILE:HD11 | 1:23:A:LEU:HB3 | 15       | 0.11          |
| (1,398) | 1:15:A:ILE:HD12 | 1:23:A:LEU:HB2 | 15       | 0.11          |
| (1,398) | 1:15:A:ILE:HD12 | 1:23:A:LEU:HB3 | 15       | 0.11          |
| (1,398) | 1:15:A:ILE:HD13 | 1:23:A:LEU:HB2 | 15       | 0.11          |
| (1,398) | 1:15:A:ILE:HD13 | 1:23:A:LEU:HB3 | 15       | 0.11          |
| (1,387) | 1:15:A:ILE:HD11 | 1:19:A:ASP:H   | 17       | 0.11          |
| (1,387) | 1:15:A:ILE:HD12 | 1:19:A:ASP:H   | 17       | 0.11          |
| (1,387) | 1:15:A:ILE:HD13 | 1:19:A:ASP:H   | 17       | 0.11          |
| (1,373) | 1:14:A:ASN:HB2  | 1:75:A:LEU:HG  | 13       | 0.11          |
| (1,373) | 1:14:A:ASN:HB3  | 1:75:A:LEU:HG  | 13       | 0.11          |
| (1,373) | 1:14:A:ASN:HB2  | 1:75:A:LEU:HG  | 18       | 0.11          |
| (1,373) | 1:14:A:ASN:HB3  | 1:75:A:LEU:HG  | 18       | 0.11          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD1 | 18       | 0.11          |
| (1,339) | 1:12:A:THR:HG21 | 1:46:A:PHE:HD2 | 18       | 0.11          |
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD1 | 18       | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,339) | 1:12:A:THR:HG22 | 1:46:A:PHE:HD2  | 18       | 0.11          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD1  | 18       | 0.11          |
| (1,339) | 1:12:A:THR:HG23 | 1:46:A:PHE:HD2  | 18       | 0.11          |
| (1,335) | 1:12:A:THR:HB   | 1:42:A:GLY:H    | 15       | 0.11          |
| (1,309) | 1:11:A:LEU:HD11 | 1:78:A:MET:HB2  | 18       | 0.11          |
| (1,309) | 1:11:A:LEU:HD11 | 1:78:A:MET:HB3  | 18       | 0.11          |
| (1,309) | 1:11:A:LEU:HD12 | 1:78:A:MET:HB2  | 18       | 0.11          |
| (1,309) | 1:11:A:LEU:HD12 | 1:78:A:MET:HB3  | 18       | 0.11          |
| (1,309) | 1:11:A:LEU:HD13 | 1:78:A:MET:HB2  | 18       | 0.11          |
| (1,309) | 1:11:A:LEU:HD13 | 1:78:A:MET:HB3  | 18       | 0.11          |
| (1,309) | 1:11:A:LEU:HD21 | 1:78:A:MET:HB2  | 18       | 0.11          |
| (1,309) | 1:11:A:LEU:HD21 | 1:78:A:MET:HB3  | 18       | 0.11          |
| (1,309) | 1:11:A:LEU:HD22 | 1:78:A:MET:HB2  | 18       | 0.11          |
| (1,309) | 1:11:A:LEU:HD22 | 1:78:A:MET:HB3  | 18       | 0.11          |
| (1,309) | 1:11:A:LEU:HD23 | 1:78:A:MET:HB2  | 18       | 0.11          |
| (1,309) | 1:11:A:LEU:HD23 | 1:78:A:MET:HB3  | 18       | 0.11          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD11 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD12 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD13 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD21 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD22 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD11 | 1:55:A:LEU:HD23 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD11 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD12 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD13 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD21 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD22 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD12 | 1:55:A:LEU:HD23 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD11 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD12 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD13 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD21 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD22 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD13 | 1:55:A:LEU:HD23 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD11 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD12 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD13 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD21 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD22 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD21 | 1:55:A:LEU:HD23 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD11 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD12 | 15       | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD13 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD21 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD22 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD22 | 1:55:A:LEU:HD23 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD11 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD12 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD13 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD21 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD22 | 15       | 0.11          |
| (1,296) | 1:11:A:LEU:HD23 | 1:55:A:LEU:HD23 | 15       | 0.11          |
| (1,263) | 1:10:A:ASP:H    | 1:14:A:ASN:H    | 16       | 0.11          |
| (1,227) | 1:9:A:GLN:HG2   | 1:9:A:GLN:H     | 16       | 0.11          |
| (1,227) | 1:9:A:GLN:HG3   | 1:9:A:GLN:H     | 16       | 0.11          |
| (1,204) | 1:8:A:LEU:HB2   | 1:46:A:PHE:HE1  | 12       | 0.11          |
| (1,204) | 1:8:A:LEU:HB2   | 1:46:A:PHE:HE2  | 12       | 0.11          |
| (1,204) | 1:8:A:LEU:HB3   | 1:46:A:PHE:HE1  | 12       | 0.11          |
| (1,204) | 1:8:A:LEU:HB3   | 1:46:A:PHE:HE2  | 12       | 0.11          |
| (1,204) | 1:8:A:LEU:HB2   | 1:46:A:PHE:HE1  | 13       | 0.11          |
| (1,204) | 1:8:A:LEU:HB2   | 1:46:A:PHE:HE2  | 13       | 0.11          |
| (1,204) | 1:8:A:LEU:HB3   | 1:46:A:PHE:HE1  | 13       | 0.11          |
| (1,204) | 1:8:A:LEU:HB3   | 1:46:A:PHE:HE2  | 13       | 0.11          |
| (1,204) | 1:8:A:LEU:HB2   | 1:46:A:PHE:HE1  | 15       | 0.11          |
| (1,204) | 1:8:A:LEU:HB2   | 1:46:A:PHE:HE2  | 15       | 0.11          |
| (1,204) | 1:8:A:LEU:HB3   | 1:46:A:PHE:HE1  | 15       | 0.11          |
| (1,204) | 1:8:A:LEU:HB3   | 1:46:A:PHE:HE2  | 15       | 0.11          |
| (1,196) | 1:8:A:LEU:HD11  | 1:11:A:LEU:HB2  | 8        | 0.11          |
| (1,196) | 1:8:A:LEU:HD11  | 1:11:A:LEU:HB3  | 8        | 0.11          |
| (1,196) | 1:8:A:LEU:HD12  | 1:11:A:LEU:HB2  | 8        | 0.11          |
| (1,196) | 1:8:A:LEU:HD12  | 1:11:A:LEU:HB3  | 8        | 0.11          |
| (1,196) | 1:8:A:LEU:HD13  | 1:11:A:LEU:HB2  | 8        | 0.11          |
| (1,196) | 1:8:A:LEU:HD13  | 1:11:A:LEU:HB3  | 8        | 0.11          |
| (1,196) | 1:8:A:LEU:HD21  | 1:11:A:LEU:HB2  | 8        | 0.11          |
| (1,196) | 1:8:A:LEU:HD21  | 1:11:A:LEU:HB3  | 8        | 0.11          |
| (1,196) | 1:8:A:LEU:HD22  | 1:11:A:LEU:HB2  | 8        | 0.11          |
| (1,196) | 1:8:A:LEU:HD22  | 1:11:A:LEU:HB3  | 8        | 0.11          |
| (1,196) | 1:8:A:LEU:HD23  | 1:11:A:LEU:HB2  | 8        | 0.11          |
| (1,196) | 1:8:A:LEU:HD23  | 1:11:A:LEU:HB3  | 8        | 0.11          |
| (1,127) | 1:6:A:THR:HB    | 1:9:A:GLN:HG2   | 15       | 0.11          |
| (1,127) | 1:6:A:THR:HB    | 1:9:A:GLN:HG3   | 15       | 0.11          |
| (1,124) | 1:6:A:THR:HA    | 1:9:A:GLN:HG2   | 3        | 0.11          |
| (1,124) | 1:6:A:THR:HA    | 1:9:A:GLN:HG3   | 3        | 0.11          |
| (1,124) | 1:6:A:THR:HA    | 1:9:A:GLN:HG2   | 7        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,124)  | 1:6:A:THR:HA    | 1:9:A:GLN:HG3   | 7        | 0.11          |
| (1,124)  | 1:6:A:THR:HA    | 1:9:A:GLN:HG2   | 10       | 0.11          |
| (1,124)  | 1:6:A:THR:HA    | 1:9:A:GLN:HG3   | 10       | 0.11          |
| (1,124)  | 1:6:A:THR:HA    | 1:9:A:GLN:HG2   | 17       | 0.11          |
| (1,124)  | 1:6:A:THR:HA    | 1:9:A:GLN:HG3   | 17       | 0.11          |
| (1,93)   | 1:4:A:TYR:HA    | 1:82:A:TYR:HE1  | 2        | 0.11          |
| (1,93)   | 1:4:A:TYR:HA    | 1:82:A:TYR:HE2  | 2        | 0.11          |
| (1,76)   | 1:4:A:TYR:HD1   | 1:56:A:ASP:HA   | 16       | 0.11          |
| (1,76)   | 1:4:A:TYR:HD2   | 1:56:A:ASP:HA   | 16       | 0.11          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD11  | 2        | 0.11          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD12  | 2        | 0.11          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD13  | 2        | 0.11          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD21  | 2        | 0.11          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD22  | 2        | 0.11          |
| (1,67)   | 1:4:A:TYR:HB2   | 1:7:A:LEU:HD23  | 2        | 0.11          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD11  | 2        | 0.11          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD12  | 2        | 0.11          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD13  | 2        | 0.11          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD21  | 2        | 0.11          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD22  | 2        | 0.11          |
| (1,67)   | 1:4:A:TYR:HB3   | 1:7:A:LEU:HD23  | 2        | 0.11          |
| (1,10)   | 1:1:A:MET:HA    | 1:57:A:LYS:HD2  | 12       | 0.11          |
| (1,10)   | 1:1:A:MET:HA    | 1:57:A:LYS:HD3  | 12       | 0.11          |
| (1,10)   | 1:1:A:MET:HA    | 1:57:A:LYS:HD2  | 20       | 0.11          |
| (1,10)   | 1:1:A:MET:HA    | 1:57:A:LYS:HD3  | 20       | 0.11          |
| (1,6)    | 1:1:A:MET:HA    | 1:3:A:GLU:H     | 1        | 0.11          |
| (2,82)   | 1:83:A:ARG:O    | 1:87:A:LEU:H    | 6        | 0.1           |
| (1,1900) | 1:89:A:ILE:HG21 | 1:90:A:SER:HB2  | 4        | 0.1           |
| (1,1900) | 1:89:A:ILE:HG21 | 1:90:A:SER:HB3  | 4        | 0.1           |
| (1,1900) | 1:89:A:ILE:HG22 | 1:90:A:SER:HB2  | 4        | 0.1           |
| (1,1900) | 1:89:A:ILE:HG22 | 1:90:A:SER:HB3  | 4        | 0.1           |
| (1,1900) | 1:89:A:ILE:HG23 | 1:90:A:SER:HB2  | 4        | 0.1           |
| (1,1900) | 1:89:A:ILE:HG23 | 1:90:A:SER:HB3  | 4        | 0.1           |
| (1,1900) | 1:89:A:ILE:HG21 | 1:90:A:SER:HB2  | 7        | 0.1           |
| (1,1900) | 1:89:A:ILE:HG21 | 1:90:A:SER:HB3  | 7        | 0.1           |
| (1,1900) | 1:89:A:ILE:HG22 | 1:90:A:SER:HB2  | 7        | 0.1           |
| (1,1900) | 1:89:A:ILE:HG22 | 1:90:A:SER:HB3  | 7        | 0.1           |
| (1,1900) | 1:89:A:ILE:HG23 | 1:90:A:SER:HB2  | 7        | 0.1           |
| (1,1900) | 1:89:A:ILE:HG23 | 1:90:A:SER:HB3  | 7        | 0.1           |
| (1,1874) | 1:87:A:LEU:HB2  | 1:89:A:ILE:HG21 | 13       | 0.1           |
| (1,1874) | 1:87:A:LEU:HB2  | 1:89:A:ILE:HG22 | 13       | 0.1           |
| (1,1874) | 1:87:A:LEU:HB2  | 1:89:A:ILE:HG23 | 13       | 0.1           |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1874) | 1:87:A:LEU:HB3 | 1:89:A:ILE:HG21 | 13       | 0.1           |
| (1,1874) | 1:87:A:LEU:HB3 | 1:89:A:ILE:HG22 | 13       | 0.1           |
| (1,1874) | 1:87:A:LEU:HB3 | 1:89:A:ILE:HG23 | 13       | 0.1           |
| (1,1838) | 1:85:A:ARG:H   | 1:86:A:VAL:HB   | 7        | 0.1           |
| (1,1834) | 1:85:A:ARG:HD2 | 1:86:A:VAL:HA   | 20       | 0.1           |
| (1,1834) | 1:85:A:ARG:HD3 | 1:86:A:VAL:HA   | 20       | 0.1           |
| (1,1825) | 1:84:A:THR:HB  | 1:87:A:LEU:HG   | 1        | 0.1           |
| (1,1822) | 1:84:A:THR:HB  | 1:87:A:LEU:HD11 | 4        | 0.1           |
| (1,1822) | 1:84:A:THR:HB  | 1:87:A:LEU:HD12 | 4        | 0.1           |
| (1,1822) | 1:84:A:THR:HB  | 1:87:A:LEU:HD13 | 4        | 0.1           |
| (1,1822) | 1:84:A:THR:HB  | 1:87:A:LEU:HD21 | 4        | 0.1           |
| (1,1822) | 1:84:A:THR:HB  | 1:87:A:LEU:HD22 | 4        | 0.1           |
| (1,1822) | 1:84:A:THR:HB  | 1:87:A:LEU:HD23 | 4        | 0.1           |
| (1,1796) | 1:83:A:ARG:HD2 | 1:84:A:THR:HG21 | 3        | 0.1           |
| (1,1796) | 1:83:A:ARG:HD2 | 1:84:A:THR:HG22 | 3        | 0.1           |
| (1,1796) | 1:83:A:ARG:HD2 | 1:84:A:THR:HG23 | 3        | 0.1           |
| (1,1796) | 1:83:A:ARG:HD3 | 1:84:A:THR:HG21 | 3        | 0.1           |
| (1,1796) | 1:83:A:ARG:HD3 | 1:84:A:THR:HG22 | 3        | 0.1           |
| (1,1796) | 1:83:A:ARG:HD3 | 1:84:A:THR:HG23 | 3        | 0.1           |
| (1,1796) | 1:83:A:ARG:HD2 | 1:84:A:THR:HG21 | 12       | 0.1           |
| (1,1796) | 1:83:A:ARG:HD2 | 1:84:A:THR:HG22 | 12       | 0.1           |
| (1,1796) | 1:83:A:ARG:HD2 | 1:84:A:THR:HG23 | 12       | 0.1           |
| (1,1796) | 1:83:A:ARG:HD3 | 1:84:A:THR:HG21 | 12       | 0.1           |
| (1,1796) | 1:83:A:ARG:HD3 | 1:84:A:THR:HG22 | 12       | 0.1           |
| (1,1796) | 1:83:A:ARG:HD3 | 1:84:A:THR:HG23 | 12       | 0.1           |
| (1,1794) | 1:83:A:ARG:HG2 | 1:84:A:THR:H    | 9        | 0.1           |
| (1,1794) | 1:83:A:ARG:HG3 | 1:84:A:THR:H    | 9        | 0.1           |
| (1,1781) | 1:82:A:TYR:HB2 | 1:86:A:VAL:HG11 | 2        | 0.1           |
| (1,1781) | 1:82:A:TYR:HB2 | 1:86:A:VAL:HG12 | 2        | 0.1           |
| (1,1781) | 1:82:A:TYR:HB2 | 1:86:A:VAL:HG13 | 2        | 0.1           |
| (1,1781) | 1:82:A:TYR:HB2 | 1:86:A:VAL:HG21 | 2        | 0.1           |
| (1,1781) | 1:82:A:TYR:HB2 | 1:86:A:VAL:HG22 | 2        | 0.1           |
| (1,1781) | 1:82:A:TYR:HB2 | 1:86:A:VAL:HG23 | 2        | 0.1           |
| (1,1781) | 1:82:A:TYR:HB3 | 1:86:A:VAL:HG11 | 2        | 0.1           |
| (1,1781) | 1:82:A:TYR:HB3 | 1:86:A:VAL:HG12 | 2        | 0.1           |
| (1,1781) | 1:82:A:TYR:HB3 | 1:86:A:VAL:HG13 | 2        | 0.1           |
| (1,1781) | 1:82:A:TYR:HB3 | 1:86:A:VAL:HG21 | 2        | 0.1           |
| (1,1781) | 1:82:A:TYR:HB3 | 1:86:A:VAL:HG22 | 2        | 0.1           |
| (1,1781) | 1:82:A:TYR:HB3 | 1:86:A:VAL:HG23 | 2        | 0.1           |
| (1,1683) | 1:77:A:THR:HB  | 1:79:A:VAL:HG11 | 12       | 0.1           |
| (1,1683) | 1:77:A:THR:HB  | 1:79:A:VAL:HG12 | 12       | 0.1           |
| (1,1683) | 1:77:A:THR:HB  | 1:79:A:VAL:HG13 | 12       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG21 | 12       | 0.1           |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG22 | 12       | 0.1           |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG23 | 12       | 0.1           |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG11 | 14       | 0.1           |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG12 | 14       | 0.1           |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG13 | 14       | 0.1           |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG21 | 14       | 0.1           |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG22 | 14       | 0.1           |
| (1,1683) | 1:77:A:THR:HB   | 1:79:A:VAL:HG23 | 14       | 0.1           |
| (1,1680) | 1:77:A:THR:HG21 | 1:78:A:MET:HG2  | 13       | 0.1           |
| (1,1680) | 1:77:A:THR:HG21 | 1:78:A:MET:HG3  | 13       | 0.1           |
| (1,1680) | 1:77:A:THR:HG22 | 1:78:A:MET:HG2  | 13       | 0.1           |
| (1,1680) | 1:77:A:THR:HG22 | 1:78:A:MET:HG3  | 13       | 0.1           |
| (1,1680) | 1:77:A:THR:HG23 | 1:78:A:MET:HG2  | 13       | 0.1           |
| (1,1680) | 1:77:A:THR:HG23 | 1:78:A:MET:HG3  | 13       | 0.1           |
| (1,1576) | 1:71:A:ARG:HA   | 1:71:A:ARG:HG2  | 1        | 0.1           |
| (1,1576) | 1:71:A:ARG:HA   | 1:71:A:ARG:HG3  | 1        | 0.1           |
| (1,1576) | 1:71:A:ARG:HA   | 1:71:A:ARG:HG2  | 10       | 0.1           |
| (1,1576) | 1:71:A:ARG:HA   | 1:71:A:ARG:HG3  | 10       | 0.1           |
| (1,1576) | 1:71:A:ARG:HA   | 1:71:A:ARG:HG2  | 12       | 0.1           |
| (1,1576) | 1:71:A:ARG:HA   | 1:71:A:ARG:HG3  | 12       | 0.1           |
| (1,1576) | 1:71:A:ARG:HA   | 1:71:A:ARG:HG2  | 18       | 0.1           |
| (1,1576) | 1:71:A:ARG:HA   | 1:71:A:ARG:HG3  | 18       | 0.1           |
| (1,1547) | 1:69:A:ILE:HB   | 1:69:A:ILE:H    | 4        | 0.1           |
| (1,1538) | 1:68:A:GLU:HA   | 1:71:A:ARG:HD2  | 9        | 0.1           |
| (1,1538) | 1:68:A:GLU:HA   | 1:71:A:ARG:HD3  | 9        | 0.1           |
| (1,1538) | 1:68:A:GLU:HA   | 1:71:A:ARG:HD2  | 11       | 0.1           |
| (1,1538) | 1:68:A:GLU:HA   | 1:71:A:ARG:HD3  | 11       | 0.1           |
| (1,1516) | 1:67:A:PHE:H    | 1:76:A:LEU:HG   | 4        | 0.1           |
| (1,1516) | 1:67:A:PHE:H    | 1:76:A:LEU:HG   | 5        | 0.1           |
| (1,1468) | 1:66:A:ILE:HA   | 1:69:A:ILE:HG21 | 11       | 0.1           |
| (1,1468) | 1:66:A:ILE:HA   | 1:69:A:ILE:HG22 | 11       | 0.1           |
| (1,1468) | 1:66:A:ILE:HA   | 1:69:A:ILE:HG23 | 11       | 0.1           |
| (1,1465) | 1:66:A:ILE:HD11 | 1:69:A:ILE:HA   | 2        | 0.1           |
| (1,1465) | 1:66:A:ILE:HD12 | 1:69:A:ILE:HA   | 2        | 0.1           |
| (1,1465) | 1:66:A:ILE:HD13 | 1:69:A:ILE:HA   | 2        | 0.1           |
| (1,1461) | 1:66:A:ILE:HG21 | 1:67:A:PHE:HA   | 19       | 0.1           |
| (1,1461) | 1:66:A:ILE:HG22 | 1:67:A:PHE:HA   | 19       | 0.1           |
| (1,1461) | 1:66:A:ILE:HG23 | 1:67:A:PHE:HA   | 19       | 0.1           |
| (1,1459) | 1:66:A:ILE:HG21 | 1:67:A:PHE:HE1  | 18       | 0.1           |
| (1,1459) | 1:66:A:ILE:HG21 | 1:67:A:PHE:HE2  | 18       | 0.1           |
| (1,1459) | 1:66:A:ILE:HG22 | 1:67:A:PHE:HE1  | 18       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1459) | 1:66:A:ILE:HG22 | 1:67:A:PHE:HE2  | 18       | 0.1           |
| (1,1459) | 1:66:A:ILE:HG23 | 1:67:A:PHE:HE1  | 18       | 0.1           |
| (1,1459) | 1:66:A:ILE:HG23 | 1:67:A:PHE:HE2  | 18       | 0.1           |
| (1,1452) | 1:66:A:ILE:HA   | 1:66:A:ILE:HG12 | 5        | 0.1           |
| (1,1452) | 1:66:A:ILE:HA   | 1:66:A:ILE:HG13 | 5        | 0.1           |
| (1,1445) | 1:66:A:ILE:HG12 | 1:66:A:ILE:H    | 13       | 0.1           |
| (1,1445) | 1:66:A:ILE:HG13 | 1:66:A:ILE:H    | 13       | 0.1           |
| (1,1439) | 1:65:A:HIS:HA   | 1:69:A:ILE:H    | 17       | 0.1           |
| (1,1434) | 1:65:A:HIS:HB2  | 1:67:A:PHE:HD1  | 12       | 0.1           |
| (1,1434) | 1:65:A:HIS:HB2  | 1:67:A:PHE:HD2  | 12       | 0.1           |
| (1,1434) | 1:65:A:HIS:HB3  | 1:67:A:PHE:HD1  | 12       | 0.1           |
| (1,1434) | 1:65:A:HIS:HB3  | 1:67:A:PHE:HD2  | 12       | 0.1           |
| (1,1379) | 1:63:A:ILE:HD11 | 1:67:A:PHE:H    | 5        | 0.1           |
| (1,1379) | 1:63:A:ILE:HD12 | 1:67:A:PHE:H    | 5        | 0.1           |
| (1,1379) | 1:63:A:ILE:HD13 | 1:67:A:PHE:H    | 5        | 0.1           |
| (1,1346) | 1:62:A:TYR:H    | 1:66:A:ILE:HD11 | 7        | 0.1           |
| (1,1346) | 1:62:A:TYR:H    | 1:66:A:ILE:HD12 | 7        | 0.1           |
| (1,1346) | 1:62:A:TYR:H    | 1:66:A:ILE:HD13 | 7        | 0.1           |
| (1,1336) | 1:62:A:TYR:HD1  | 1:63:A:ILE:HG21 | 15       | 0.1           |
| (1,1336) | 1:62:A:TYR:HD1  | 1:63:A:ILE:HG22 | 15       | 0.1           |
| (1,1336) | 1:62:A:TYR:HD1  | 1:63:A:ILE:HG23 | 15       | 0.1           |
| (1,1336) | 1:62:A:TYR:HD2  | 1:63:A:ILE:HG21 | 15       | 0.1           |
| (1,1336) | 1:62:A:TYR:HD2  | 1:63:A:ILE:HG22 | 15       | 0.1           |
| (1,1336) | 1:62:A:TYR:HD2  | 1:63:A:ILE:HG23 | 15       | 0.1           |
| (1,1324) | 1:61:A:SER:H    | 1:65:A:HIS:H    | 12       | 0.1           |
| (1,1319) | 1:61:A:SER:HA   | 1:63:A:ILE:HG21 | 18       | 0.1           |
| (1,1319) | 1:61:A:SER:HA   | 1:63:A:ILE:HG22 | 18       | 0.1           |
| (1,1319) | 1:61:A:SER:HA   | 1:63:A:ILE:HG23 | 18       | 0.1           |
| (1,1292) | 1:60:A:LEU:HA   | 1:60:A:LEU:HD11 | 16       | 0.1           |
| (1,1292) | 1:60:A:LEU:HA   | 1:60:A:LEU:HD12 | 16       | 0.1           |
| (1,1292) | 1:60:A:LEU:HA   | 1:60:A:LEU:HD13 | 16       | 0.1           |
| (1,1292) | 1:60:A:LEU:HA   | 1:60:A:LEU:HD21 | 16       | 0.1           |
| (1,1292) | 1:60:A:LEU:HA   | 1:60:A:LEU:HD22 | 16       | 0.1           |
| (1,1292) | 1:60:A:LEU:HA   | 1:60:A:LEU:HD23 | 16       | 0.1           |
| (1,1274) | 1:58:A:ASP:H    | 1:59:A:ASN:HD21 | 8        | 0.1           |
| (1,1274) | 1:58:A:ASP:H    | 1:59:A:ASN:HD22 | 8        | 0.1           |
| (1,1273) | 1:58:A:ASP:HA   | 1:59:A:ASN:HD21 | 15       | 0.1           |
| (1,1273) | 1:58:A:ASP:HA   | 1:59:A:ASN:HD22 | 15       | 0.1           |
| (1,1255) | 1:57:A:LYS:HA   | 1:57:A:LYS:HG2  | 16       | 0.1           |
| (1,1255) | 1:57:A:LYS:HA   | 1:57:A:LYS:HG3  | 16       | 0.1           |
| (1,1241) | 1:56:A:ASP:HB2  | 1:57:A:LYS:H    | 4        | 0.1           |
| (1,1241) | 1:56:A:ASP:HB3  | 1:57:A:LYS:H    | 4        | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1230) | 1:55:A:LEU:HD11 | 1:60:A:LEU:HA   | 9        | 0.1           |
| (1,1230) | 1:55:A:LEU:HD12 | 1:60:A:LEU:HA   | 9        | 0.1           |
| (1,1230) | 1:55:A:LEU:HD13 | 1:60:A:LEU:HA   | 9        | 0.1           |
| (1,1230) | 1:55:A:LEU:HD21 | 1:60:A:LEU:HA   | 9        | 0.1           |
| (1,1230) | 1:55:A:LEU:HD22 | 1:60:A:LEU:HA   | 9        | 0.1           |
| (1,1230) | 1:55:A:LEU:HD23 | 1:60:A:LEU:HA   | 9        | 0.1           |
| (1,1230) | 1:55:A:LEU:HD11 | 1:60:A:LEU:HA   | 19       | 0.1           |
| (1,1230) | 1:55:A:LEU:HD12 | 1:60:A:LEU:HA   | 19       | 0.1           |
| (1,1230) | 1:55:A:LEU:HD13 | 1:60:A:LEU:HA   | 19       | 0.1           |
| (1,1230) | 1:55:A:LEU:HD21 | 1:60:A:LEU:HA   | 19       | 0.1           |
| (1,1230) | 1:55:A:LEU:HD22 | 1:60:A:LEU:HA   | 19       | 0.1           |
| (1,1230) | 1:55:A:LEU:HD23 | 1:60:A:LEU:HA   | 19       | 0.1           |
| (1,1228) | 1:55:A:LEU:HG   | 1:59:A:ASN:HD21 | 18       | 0.1           |
| (1,1228) | 1:55:A:LEU:HG   | 1:59:A:ASN:HD22 | 18       | 0.1           |
| (1,1207) | 1:54:A:LYS:HG2  | 1:62:A:TYR:HE1  | 1        | 0.1           |
| (1,1207) | 1:54:A:LYS:HG2  | 1:62:A:TYR:HE2  | 1        | 0.1           |
| (1,1207) | 1:54:A:LYS:HG3  | 1:62:A:TYR:HE1  | 1        | 0.1           |
| (1,1207) | 1:54:A:LYS:HG3  | 1:62:A:TYR:HE2  | 1        | 0.1           |
| (1,1207) | 1:54:A:LYS:HG2  | 1:62:A:TYR:HE1  | 8        | 0.1           |
| (1,1207) | 1:54:A:LYS:HG2  | 1:62:A:TYR:HE2  | 8        | 0.1           |
| (1,1207) | 1:54:A:LYS:HG3  | 1:62:A:TYR:HE1  | 8        | 0.1           |
| (1,1207) | 1:54:A:LYS:HG3  | 1:62:A:TYR:HE2  | 8        | 0.1           |
| (1,1207) | 1:54:A:LYS:HG2  | 1:62:A:TYR:HE1  | 15       | 0.1           |
| (1,1207) | 1:54:A:LYS:HG2  | 1:62:A:TYR:HE2  | 15       | 0.1           |
| (1,1207) | 1:54:A:LYS:HG3  | 1:62:A:TYR:HE1  | 15       | 0.1           |
| (1,1207) | 1:54:A:LYS:HG3  | 1:62:A:TYR:HE2  | 15       | 0.1           |
| (1,1206) | 1:54:A:LYS:HB2  | 1:62:A:TYR:HE1  | 9        | 0.1           |
| (1,1206) | 1:54:A:LYS:HB2  | 1:62:A:TYR:HE2  | 9        | 0.1           |
| (1,1206) | 1:54:A:LYS:HB3  | 1:62:A:TYR:HE1  | 9        | 0.1           |
| (1,1206) | 1:54:A:LYS:HB3  | 1:62:A:TYR:HE2  | 9        | 0.1           |
| (1,1194) | 1:54:A:LYS:HD2  | 1:54:A:LYS:H    | 4        | 0.1           |
| (1,1194) | 1:54:A:LYS:HD3  | 1:54:A:LYS:H    | 4        | 0.1           |
| (1,1194) | 1:54:A:LYS:HD2  | 1:54:A:LYS:H    | 13       | 0.1           |
| (1,1194) | 1:54:A:LYS:HD3  | 1:54:A:LYS:H    | 13       | 0.1           |
| (1,1193) | 1:53:A:ASN:H    | 1:55:A:LEU:H    | 1        | 0.1           |
| (1,1193) | 1:53:A:ASN:H    | 1:55:A:LEU:H    | 3        | 0.1           |
| (1,1193) | 1:53:A:ASN:H    | 1:55:A:LEU:H    | 10       | 0.1           |
| (1,1193) | 1:53:A:ASN:H    | 1:55:A:LEU:H    | 17       | 0.1           |
| (1,1193) | 1:53:A:ASN:H    | 1:55:A:LEU:H    | 18       | 0.1           |
| (1,1193) | 1:53:A:ASN:H    | 1:55:A:LEU:H    | 19       | 0.1           |
| (1,1132) | 1:49:A:LEU:HD11 | 1:63:A:ILE:HB   | 17       | 0.1           |
| (1,1132) | 1:49:A:LEU:HD12 | 1:63:A:ILE:HB   | 17       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1132) | 1:49:A:LEU:HD13 | 1:63:A:ILE:HB   | 17       | 0.1           |
| (1,1132) | 1:49:A:LEU:HD21 | 1:63:A:ILE:HB   | 17       | 0.1           |
| (1,1132) | 1:49:A:LEU:HD22 | 1:63:A:ILE:HB   | 17       | 0.1           |
| (1,1132) | 1:49:A:LEU:HD23 | 1:63:A:ILE:HB   | 17       | 0.1           |
| (1,1128) | 1:49:A:LEU:HD11 | 1:62:A:TYR:HE1  | 8        | 0.1           |
| (1,1128) | 1:49:A:LEU:HD11 | 1:62:A:TYR:HE2  | 8        | 0.1           |
| (1,1128) | 1:49:A:LEU:HD12 | 1:62:A:TYR:HE1  | 8        | 0.1           |
| (1,1128) | 1:49:A:LEU:HD12 | 1:62:A:TYR:HE2  | 8        | 0.1           |
| (1,1128) | 1:49:A:LEU:HD13 | 1:62:A:TYR:HE1  | 8        | 0.1           |
| (1,1128) | 1:49:A:LEU:HD13 | 1:62:A:TYR:HE2  | 8        | 0.1           |
| (1,1128) | 1:49:A:LEU:HD21 | 1:62:A:TYR:HE1  | 8        | 0.1           |
| (1,1128) | 1:49:A:LEU:HD21 | 1:62:A:TYR:HE2  | 8        | 0.1           |
| (1,1128) | 1:49:A:LEU:HD22 | 1:62:A:TYR:HE1  | 8        | 0.1           |
| (1,1128) | 1:49:A:LEU:HD22 | 1:62:A:TYR:HE2  | 8        | 0.1           |
| (1,1128) | 1:49:A:LEU:HD23 | 1:62:A:TYR:HE1  | 8        | 0.1           |
| (1,1128) | 1:49:A:LEU:HD23 | 1:62:A:TYR:HE2  | 8        | 0.1           |
| (1,1112) | 1:49:A:LEU:HA   | 1:54:A:LYS:HA   | 16       | 0.1           |
| (1,1062) | 1:47:A:SER:HA   | 1:51:A:SER:H    | 18       | 0.1           |
| (1,1018) | 1:46:A:PHE:HD1  | 1:46:A:PHE:H    | 2        | 0.1           |
| (1,1018) | 1:46:A:PHE:HD2  | 1:46:A:PHE:H    | 2        | 0.1           |
| (1,1018) | 1:46:A:PHE:HD1  | 1:46:A:PHE:H    | 18       | 0.1           |
| (1,1018) | 1:46:A:PHE:HD2  | 1:46:A:PHE:H    | 18       | 0.1           |
| (1,932)  | 1:41:A:THR:HB   | 1:44:A:ALA:HB1  | 6        | 0.1           |
| (1,932)  | 1:41:A:THR:HB   | 1:44:A:ALA:HB2  | 6        | 0.1           |
| (1,932)  | 1:41:A:THR:HB   | 1:44:A:ALA:HB3  | 6        | 0.1           |
| (1,926)  | 1:41:A:THR:HB   | 1:42:A:GLY:H    | 1        | 0.1           |
| (1,926)  | 1:41:A:THR:HB   | 1:42:A:GLY:H    | 7        | 0.1           |
| (1,923)  | 1:41:A:THR:HB   | 1:41:A:THR:H    | 8        | 0.1           |
| (1,923)  | 1:41:A:THR:HB   | 1:41:A:THR:H    | 12       | 0.1           |
| (1,923)  | 1:41:A:THR:HB   | 1:41:A:THR:H    | 18       | 0.1           |
| (1,855)  | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD11 | 9        | 0.1           |
| (1,855)  | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD12 | 9        | 0.1           |
| (1,855)  | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD13 | 9        | 0.1           |
| (1,855)  | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD11 | 9        | 0.1           |
| (1,855)  | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD12 | 9        | 0.1           |
| (1,855)  | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD13 | 9        | 0.1           |
| (1,855)  | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD11 | 16       | 0.1           |
| (1,855)  | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD12 | 16       | 0.1           |
| (1,855)  | 1:38:A:GLU:HG2  | 1:39:A:ILE:HD13 | 16       | 0.1           |
| (1,855)  | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD11 | 16       | 0.1           |
| (1,855)  | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD12 | 16       | 0.1           |
| (1,855)  | 1:38:A:GLU:HG3  | 1:39:A:ILE:HD13 | 16       | 0.1           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,839) | 1:36:A:SER:HB2  | 1:39:A:ILE:HD11 | 7        | 0.1           |
| (1,839) | 1:36:A:SER:HB2  | 1:39:A:ILE:HD12 | 7        | 0.1           |
| (1,839) | 1:36:A:SER:HB2  | 1:39:A:ILE:HD13 | 7        | 0.1           |
| (1,839) | 1:36:A:SER:HB3  | 1:39:A:ILE:HD11 | 7        | 0.1           |
| (1,839) | 1:36:A:SER:HB3  | 1:39:A:ILE:HD12 | 7        | 0.1           |
| (1,839) | 1:36:A:SER:HB3  | 1:39:A:ILE:HD13 | 7        | 0.1           |
| (1,802) | 1:35:A:LYS:HA   | 1:35:A:LYS:HD2  | 17       | 0.1           |
| (1,802) | 1:35:A:LYS:HA   | 1:35:A:LYS:HD3  | 17       | 0.1           |
| (1,783) | 1:32:A:PRO:HD2  | 1:35:A:LYS:HG2  | 16       | 0.1           |
| (1,783) | 1:32:A:PRO:HD2  | 1:35:A:LYS:HG3  | 16       | 0.1           |
| (1,783) | 1:32:A:PRO:HD3  | 1:35:A:LYS:HG2  | 16       | 0.1           |
| (1,783) | 1:32:A:PRO:HD3  | 1:35:A:LYS:HG3  | 16       | 0.1           |
| (1,767) | 1:31:A:ILE:HG12 | 1:48:A:PHE:HE1  | 6        | 0.1           |
| (1,767) | 1:31:A:ILE:HG12 | 1:48:A:PHE:HE2  | 6        | 0.1           |
| (1,767) | 1:31:A:ILE:HG13 | 1:48:A:PHE:HE1  | 6        | 0.1           |
| (1,767) | 1:31:A:ILE:HG13 | 1:48:A:PHE:HE2  | 6        | 0.1           |
| (1,765) | 1:31:A:ILE:HG12 | 1:48:A:PHE:HD1  | 16       | 0.1           |
| (1,765) | 1:31:A:ILE:HG12 | 1:48:A:PHE:HD2  | 16       | 0.1           |
| (1,765) | 1:31:A:ILE:HG13 | 1:48:A:PHE:HD1  | 16       | 0.1           |
| (1,765) | 1:31:A:ILE:HG13 | 1:48:A:PHE:HD2  | 16       | 0.1           |
| (1,761) | 1:31:A:ILE:HD11 | 1:45:A:TRP:HD1  | 9        | 0.1           |
| (1,761) | 1:31:A:ILE:HD12 | 1:45:A:TRP:HD1  | 9        | 0.1           |
| (1,761) | 1:31:A:ILE:HD13 | 1:45:A:TRP:HD1  | 9        | 0.1           |
| (1,736) | 1:31:A:ILE:HB   | 1:32:A:PRO:HA   | 8        | 0.1           |
| (1,736) | 1:31:A:ILE:HB   | 1:32:A:PRO:HA   | 19       | 0.1           |
| (1,724) | 1:31:A:ILE:HD11 | 1:31:A:ILE:H    | 6        | 0.1           |
| (1,724) | 1:31:A:ILE:HD12 | 1:31:A:ILE:H    | 6        | 0.1           |
| (1,724) | 1:31:A:ILE:HD13 | 1:31:A:ILE:H    | 6        | 0.1           |
| (1,724) | 1:31:A:ILE:HD11 | 1:31:A:ILE:H    | 8        | 0.1           |
| (1,724) | 1:31:A:ILE:HD12 | 1:31:A:ILE:H    | 8        | 0.1           |
| (1,724) | 1:31:A:ILE:HD13 | 1:31:A:ILE:H    | 8        | 0.1           |
| (1,713) | 1:29:A:GLU:HB2  | 1:31:A:ILE:H    | 13       | 0.1           |
| (1,713) | 1:29:A:GLU:HB3  | 1:31:A:ILE:H    | 13       | 0.1           |
| (1,713) | 1:29:A:GLU:HB2  | 1:31:A:ILE:H    | 19       | 0.1           |
| (1,713) | 1:29:A:GLU:HB3  | 1:31:A:ILE:H    | 19       | 0.1           |
| (1,705) | 1:29:A:GLU:HA   | 1:29:A:GLU:HG2  | 4        | 0.1           |
| (1,705) | 1:29:A:GLU:HA   | 1:29:A:GLU:HG3  | 4        | 0.1           |
| (1,705) | 1:29:A:GLU:HA   | 1:29:A:GLU:HG2  | 17       | 0.1           |
| (1,705) | 1:29:A:GLU:HA   | 1:29:A:GLU:HG3  | 17       | 0.1           |
| (1,675) | 1:27:A:CYS:H    | 1:31:A:ILE:HB   | 9        | 0.1           |
| (1,675) | 1:27:A:CYS:H    | 1:31:A:ILE:HB   | 14       | 0.1           |
| (1,643) | 1:26:A:ALA:HA   | 1:28:A:LYS:HB2  | 5        | 0.1           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,643) | 1:26:A:ALA:HA   | 1:28:A:LYS:HB3  | 5        | 0.1           |
| (1,643) | 1:26:A:ALA:HA   | 1:28:A:LYS:HB2  | 16       | 0.1           |
| (1,643) | 1:26:A:ALA:HA   | 1:28:A:LYS:HB3  | 16       | 0.1           |
| (1,639) | 1:26:A:ALA:HA   | 1:27:A:CYS:H    | 17       | 0.1           |
| (1,633) | 1:25:A:SER:HA   | 1:28:A:LYS:H    | 11       | 0.1           |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG21 | 2        | 0.1           |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG22 | 2        | 0.1           |
| (1,604) | 1:23:A:LEU:HG   | 1:66:A:ILE:HG23 | 2        | 0.1           |
| (1,557) | 1:22:A:GLN:HE21 | 1:23:A:LEU:HA   | 15       | 0.1           |
| (1,557) | 1:22:A:GLN:HE22 | 1:23:A:LEU:HA   | 15       | 0.1           |
| (1,526) | 1:20:A:LEU:HD11 | 1:45:A:TRP:HZ3  | 5        | 0.1           |
| (1,526) | 1:20:A:LEU:HD12 | 1:45:A:TRP:HZ3  | 5        | 0.1           |
| (1,526) | 1:20:A:LEU:HD13 | 1:45:A:TRP:HZ3  | 5        | 0.1           |
| (1,526) | 1:20:A:LEU:HD21 | 1:45:A:TRP:HZ3  | 5        | 0.1           |
| (1,526) | 1:20:A:LEU:HD22 | 1:45:A:TRP:HZ3  | 5        | 0.1           |
| (1,526) | 1:20:A:LEU:HD23 | 1:45:A:TRP:HZ3  | 5        | 0.1           |
| (1,490) | 1:20:A:LEU:HA   | 1:20:A:LEU:HG   | 13       | 0.1           |
| (1,476) | 1:19:A:ASP:H    | 1:20:A:LEU:H    | 17       | 0.1           |
| (1,459) | 1:17:A:LEU:HG   | 1:40:A:THR:HB   | 20       | 0.1           |
| (1,405) | 1:15:A:ILE:HD11 | 1:43:A:SER:H    | 16       | 0.1           |
| (1,405) | 1:15:A:ILE:HD12 | 1:43:A:SER:H    | 16       | 0.1           |
| (1,405) | 1:15:A:ILE:HD13 | 1:43:A:SER:H    | 16       | 0.1           |
| (1,387) | 1:15:A:ILE:HD11 | 1:19:A:ASP:H    | 11       | 0.1           |
| (1,387) | 1:15:A:ILE:HD12 | 1:19:A:ASP:H    | 11       | 0.1           |
| (1,387) | 1:15:A:ILE:HD13 | 1:19:A:ASP:H    | 11       | 0.1           |
| (1,373) | 1:14:A:ASN:HB2  | 1:75:A:LEU:HG   | 11       | 0.1           |
| (1,373) | 1:14:A:ASN:HB3  | 1:75:A:LEU:HG   | 11       | 0.1           |
| (1,338) | 1:12:A:THR:HG21 | 1:46:A:PHE:HE1  | 5        | 0.1           |
| (1,338) | 1:12:A:THR:HG21 | 1:46:A:PHE:HE2  | 5        | 0.1           |
| (1,338) | 1:12:A:THR:HG22 | 1:46:A:PHE:HE1  | 5        | 0.1           |
| (1,338) | 1:12:A:THR:HG22 | 1:46:A:PHE:HE2  | 5        | 0.1           |
| (1,338) | 1:12:A:THR:HG23 | 1:46:A:PHE:HE1  | 5        | 0.1           |
| (1,338) | 1:12:A:THR:HG23 | 1:46:A:PHE:HE2  | 5        | 0.1           |
| (1,338) | 1:12:A:THR:HG21 | 1:46:A:PHE:HE1  | 6        | 0.1           |
| (1,338) | 1:12:A:THR:HG21 | 1:46:A:PHE:HE2  | 6        | 0.1           |
| (1,338) | 1:12:A:THR:HG22 | 1:46:A:PHE:HE1  | 6        | 0.1           |
| (1,338) | 1:12:A:THR:HG22 | 1:46:A:PHE:HE2  | 6        | 0.1           |
| (1,338) | 1:12:A:THR:HG23 | 1:46:A:PHE:HE1  | 6        | 0.1           |
| (1,338) | 1:12:A:THR:HG23 | 1:46:A:PHE:HE2  | 6        | 0.1           |
| (1,309) | 1:11:A:LEU:HD11 | 1:78:A:MET:HB2  | 9        | 0.1           |
| (1,309) | 1:11:A:LEU:HD11 | 1:78:A:MET:HB3  | 9        | 0.1           |
| (1,309) | 1:11:A:LEU:HD12 | 1:78:A:MET:HB2  | 9        | 0.1           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,309) | 1:11:A:LEU:HD12 | 1:78:A:MET:HB3  | 9        | 0.1           |
| (1,309) | 1:11:A:LEU:HD13 | 1:78:A:MET:HB2  | 9        | 0.1           |
| (1,309) | 1:11:A:LEU:HD13 | 1:78:A:MET:HB3  | 9        | 0.1           |
| (1,309) | 1:11:A:LEU:HD21 | 1:78:A:MET:HB2  | 9        | 0.1           |
| (1,309) | 1:11:A:LEU:HD21 | 1:78:A:MET:HB3  | 9        | 0.1           |
| (1,309) | 1:11:A:LEU:HD22 | 1:78:A:MET:HB2  | 9        | 0.1           |
| (1,309) | 1:11:A:LEU:HD22 | 1:78:A:MET:HB3  | 9        | 0.1           |
| (1,309) | 1:11:A:LEU:HD23 | 1:78:A:MET:HB2  | 9        | 0.1           |
| (1,309) | 1:11:A:LEU:HD23 | 1:78:A:MET:HB3  | 9        | 0.1           |
| (1,304) | 1:11:A:LEU:HD11 | 1:75:A:LEU:HG   | 16       | 0.1           |
| (1,304) | 1:11:A:LEU:HD12 | 1:75:A:LEU:HG   | 16       | 0.1           |
| (1,304) | 1:11:A:LEU:HD13 | 1:75:A:LEU:HG   | 16       | 0.1           |
| (1,304) | 1:11:A:LEU:HD21 | 1:75:A:LEU:HG   | 16       | 0.1           |
| (1,304) | 1:11:A:LEU:HD22 | 1:75:A:LEU:HG   | 16       | 0.1           |
| (1,304) | 1:11:A:LEU:HD23 | 1:75:A:LEU:HG   | 16       | 0.1           |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG21 | 1        | 0.1           |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG22 | 1        | 0.1           |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG23 | 1        | 0.1           |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG21 | 1        | 0.1           |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG22 | 1        | 0.1           |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG23 | 1        | 0.1           |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG21 | 2        | 0.1           |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG22 | 2        | 0.1           |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG23 | 2        | 0.1           |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG21 | 2        | 0.1           |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG22 | 2        | 0.1           |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG23 | 2        | 0.1           |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG21 | 6        | 0.1           |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG22 | 6        | 0.1           |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG23 | 6        | 0.1           |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG21 | 6        | 0.1           |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG22 | 6        | 0.1           |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG23 | 6        | 0.1           |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG21 | 16       | 0.1           |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG22 | 16       | 0.1           |
| (1,285) | 1:11:A:LEU:HB2  | 1:15:A:ILE:HG23 | 16       | 0.1           |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG21 | 16       | 0.1           |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG22 | 16       | 0.1           |
| (1,285) | 1:11:A:LEU:HB3  | 1:15:A:ILE:HG23 | 16       | 0.1           |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG21 | 16       | 0.1           |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG22 | 16       | 0.1           |
| (1,245) | 1:9:A:GLN:HE21  | 1:12:A:THR:HG23 | 16       | 0.1           |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,245) | 1:9:A:GLN:HE22 | 1:12:A:THR:HG21 | 16       | 0.1           |
| (1,245) | 1:9:A:GLN:HE22 | 1:12:A:THR:HG22 | 16       | 0.1           |
| (1,245) | 1:9:A:GLN:HE22 | 1:12:A:THR:HG23 | 16       | 0.1           |
| (1,204) | 1:8:A:LEU:HB2  | 1:46:A:PHE:HE1  | 7        | 0.1           |
| (1,204) | 1:8:A:LEU:HB2  | 1:46:A:PHE:HE2  | 7        | 0.1           |
| (1,204) | 1:8:A:LEU:HB3  | 1:46:A:PHE:HE1  | 7        | 0.1           |
| (1,204) | 1:8:A:LEU:HB3  | 1:46:A:PHE:HE2  | 7        | 0.1           |
| (1,124) | 1:6:A:THR:HA   | 1:9:A:GLN:HG2   | 2        | 0.1           |
| (1,124) | 1:6:A:THR:HA   | 1:9:A:GLN:HG3   | 2        | 0.1           |
| (1,93)  | 1:4:A:TYR:HA   | 1:82:A:TYR:HE1  | 20       | 0.1           |
| (1,93)  | 1:4:A:TYR:HA   | 1:82:A:TYR:HE2  | 20       | 0.1           |
| (1,80)  | 1:4:A:TYR:HD1  | 1:57:A:LYS:HB2  | 19       | 0.1           |
| (1,80)  | 1:4:A:TYR:HD1  | 1:57:A:LYS:HB3  | 19       | 0.1           |
| (1,80)  | 1:4:A:TYR:HD2  | 1:57:A:LYS:HB2  | 19       | 0.1           |
| (1,80)  | 1:4:A:TYR:HD2  | 1:57:A:LYS:HB3  | 19       | 0.1           |
| (1,76)  | 1:4:A:TYR:HD1  | 1:56:A:ASP:HA   | 2        | 0.1           |
| (1,76)  | 1:4:A:TYR:HD2  | 1:56:A:ASP:HA   | 2        | 0.1           |
| (1,76)  | 1:4:A:TYR:HD1  | 1:56:A:ASP:HA   | 13       | 0.1           |
| (1,76)  | 1:4:A:TYR:HD2  | 1:56:A:ASP:HA   | 13       | 0.1           |
| (1,67)  | 1:4:A:TYR:HB2  | 1:7:A:LEU:HD11  | 12       | 0.1           |
| (1,67)  | 1:4:A:TYR:HB2  | 1:7:A:LEU:HD12  | 12       | 0.1           |
| (1,67)  | 1:4:A:TYR:HB2  | 1:7:A:LEU:HD13  | 12       | 0.1           |
| (1,67)  | 1:4:A:TYR:HB2  | 1:7:A:LEU:HD21  | 12       | 0.1           |
| (1,67)  | 1:4:A:TYR:HB2  | 1:7:A:LEU:HD22  | 12       | 0.1           |
| (1,67)  | 1:4:A:TYR:HB2  | 1:7:A:LEU:HD23  | 12       | 0.1           |
| (1,67)  | 1:4:A:TYR:HB3  | 1:7:A:LEU:HD11  | 12       | 0.1           |
| (1,67)  | 1:4:A:TYR:HB3  | 1:7:A:LEU:HD12  | 12       | 0.1           |
| (1,67)  | 1:4:A:TYR:HB3  | 1:7:A:LEU:HD13  | 12       | 0.1           |
| (1,67)  | 1:4:A:TYR:HB3  | 1:7:A:LEU:HD21  | 12       | 0.1           |
| (1,67)  | 1:4:A:TYR:HB3  | 1:7:A:LEU:HD22  | 12       | 0.1           |
| (1,67)  | 1:4:A:TYR:HB3  | 1:7:A:LEU:HD23  | 12       | 0.1           |

## 10 Dihedral-angle violation analysis [i](#)

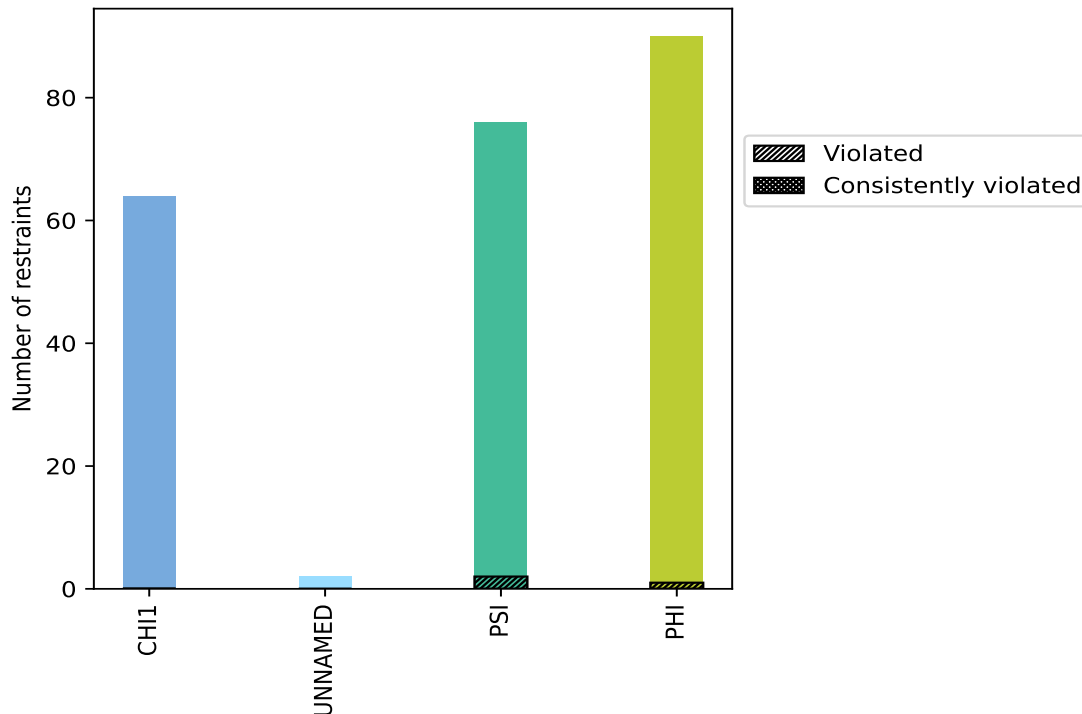
### 10.1 Summary of dihedral-angle violations [i](#)

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> |
| CHI1       | 64    | 27.6           | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| UNNAMED    | 2     | 0.9            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| PSI        | 76    | 32.8           | 2                     | 2.6            | 0.9            | 0                                  | 0.0            | 0.0            |
| PHI        | 90    | 38.8           | 1                     | 1.1            | 0.4            | 0                                  | 0.0            | 0.0            |
| Total      | 232   | 100.0          | 3                     | 1.3            | 1.3            | 0                                  | 0.0            | 0.0            |

<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](#)



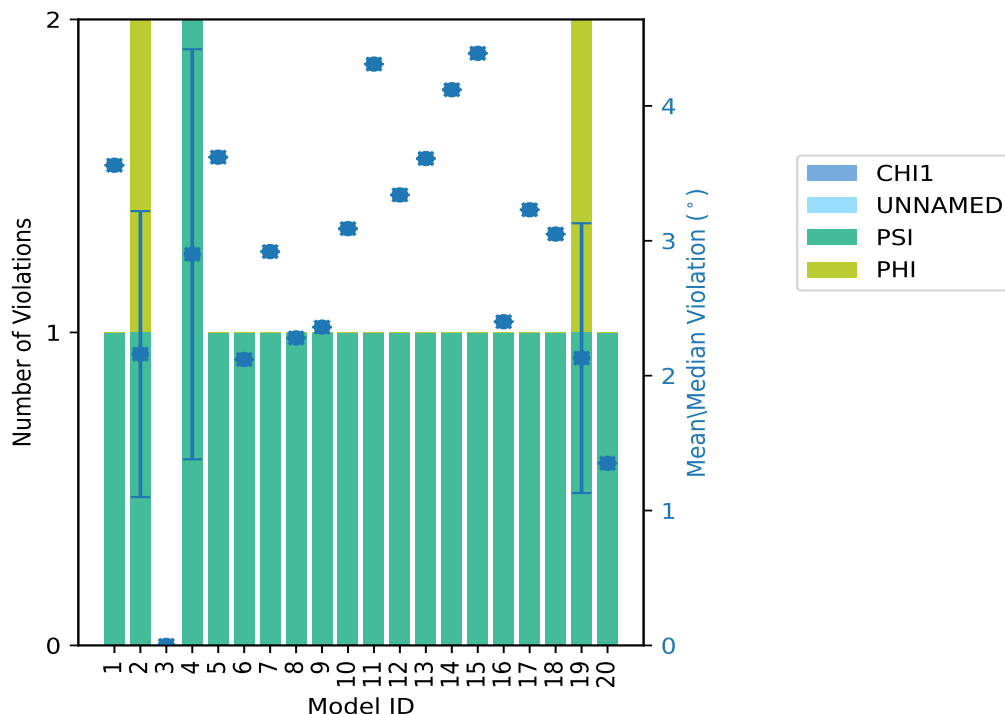
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model [\(i\)](#)

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 (°) |
|----------|----------------------|---------|-----|-----|-------|----------|---------|--------|------------|
|          | CHI1                 | UNNAMED | PSI | PHI | Total |          |         |        |            |
| 1        | 0                    | 0       | 1   | 0   | 1     | 3.56     | 3.56    | 0.0    | 3.56       |
| 2        | 0                    | 0       | 1   | 1   | 2     | 2.16     | 3.22    | 1.06   | 2.16       |
| 3        | 0                    | 0       | 0   | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 4        | 0                    | 0       | 2   | 0   | 2     | 2.9      | 4.42    | 1.52   | 2.9        |
| 5        | 0                    | 0       | 1   | 0   | 1     | 3.62     | 3.62    | 0.0    | 3.62       |
| 6        | 0                    | 0       | 1   | 0   | 1     | 2.12     | 2.12    | 0.0    | 2.12       |
| 7        | 0                    | 0       | 1   | 0   | 1     | 2.92     | 2.92    | 0.0    | 2.92       |
| 8        | 0                    | 0       | 1   | 0   | 1     | 2.28     | 2.28    | 0.0    | 2.28       |
| 9        | 0                    | 0       | 1   | 0   | 1     | 2.36     | 2.36    | 0.0    | 2.36       |
| 10       | 0                    | 0       | 1   | 0   | 1     | 3.09     | 3.09    | 0.0    | 3.09       |
| 11       | 0                    | 0       | 1   | 0   | 1     | 4.31     | 4.31    | 0.0    | 4.31       |
| 12       | 0                    | 0       | 1   | 0   | 1     | 3.34     | 3.34    | 0.0    | 3.34       |
| 13       | 0                    | 0       | 1   | 0   | 1     | 3.61     | 3.61    | 0.0    | 3.61       |
| 14       | 0                    | 0       | 1   | 0   | 1     | 4.12     | 4.12    | 0.0    | 4.12       |
| 15       | 0                    | 0       | 1   | 0   | 1     | 4.39     | 4.39    | 0.0    | 4.39       |
| 16       | 0                    | 0       | 1   | 0   | 1     | 2.4      | 2.4     | 0.0    | 2.4        |
| 17       | 0                    | 0       | 1   | 0   | 1     | 3.23     | 3.23    | 0.0    | 3.23       |
| 18       | 0                    | 0       | 1   | 0   | 1     | 3.05     | 3.05    | 0.0    | 3.05       |
| 19       | 0                    | 0       | 1   | 1   | 2     | 2.13     | 3.13    | 1.0    | 2.13       |
| 20       | 0                    | 0       | 1   | 0   | 1     | 1.35     | 1.35    | 0.0    | 1.35       |

### 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 |      |
|-------------------------------|---------|-----|-----|-------|--------------------------|------|
| CHI1                          | UNNAMED | PSI | PHI | Total | Count <sup>1</sup>       | %    |
| 0                             | 0       | 1   | 0   | 1     | 1                        | 5.0  |
| 0                             | 0       | 0   | 1   | 1     | 2                        | 10.0 |
| 0                             | 0       | 0   | 0   | 0     | 3                        | 15.0 |
| 0                             | 0       | 0   | 0   | 0     | 4                        | 20.0 |
| 0                             | 0       | 0   | 0   | 0     | 5                        | 25.0 |
| 0                             | 0       | 0   | 0   | 0     | 6                        | 30.0 |
| 0                             | 0       | 0   | 0   | 0     | 7                        | 35.0 |
| 0                             | 0       | 0   | 0   | 0     | 8                        | 40.0 |
| 0                             | 0       | 0   | 0   | 0     | 9                        | 45.0 |
| 0                             | 0       | 0   | 0   | 0     | 10                       | 50.0 |
| 0                             | 0       | 0   | 0   | 0     | 11                       | 55.0 |

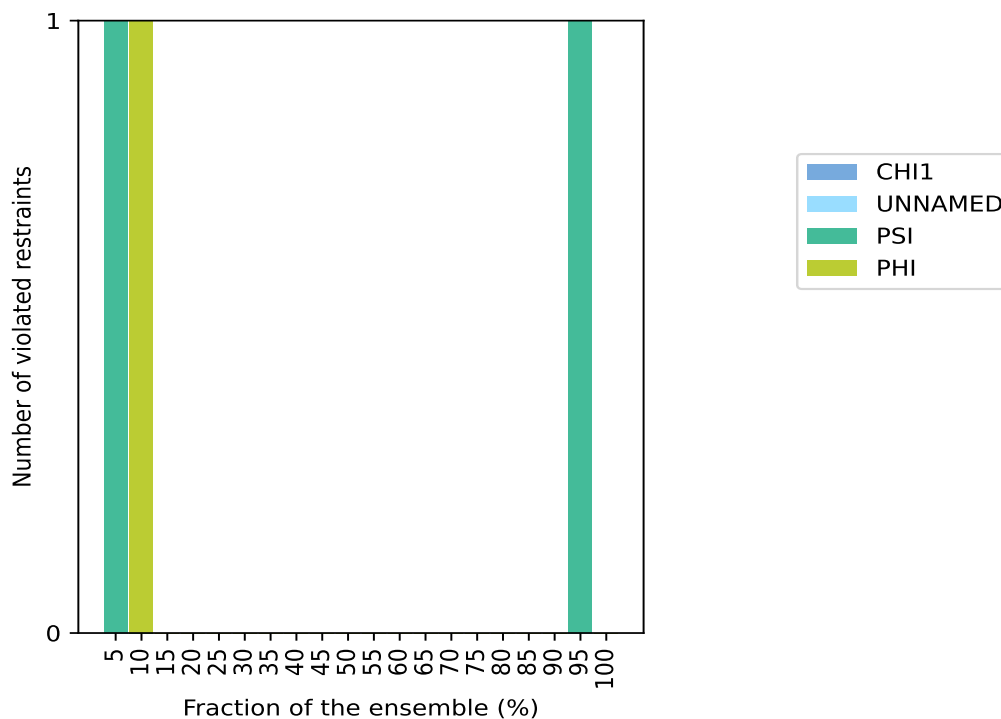
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| Number of violated restraints |         |     |     |       | Fraction of the ensemble |       |
|-------------------------------|---------|-----|-----|-------|--------------------------|-------|
| CHI1                          | UNNAMED | PSI | PHI | Total | Count <sup>1</sup>       | %     |
| 0                             | 0       | 0   | 0   | 0     | 12                       | 60.0  |
| 0                             | 0       | 0   | 0   | 0     | 13                       | 65.0  |
| 0                             | 0       | 0   | 0   | 0     | 14                       | 70.0  |
| 0                             | 0       | 0   | 0   | 0     | 15                       | 75.0  |
| 0                             | 0       | 0   | 0   | 0     | 16                       | 80.0  |
| 0                             | 0       | 0   | 0   | 0     | 17                       | 85.0  |
| 0                             | 0       | 0   | 0   | 0     | 18                       | 90.0  |
| 0                             | 0       | 1   | 0   | 1     | 19                       | 95.0  |
| 0                             | 0       | 0   | 0   | 0     | 20                       | 100.0 |

<sup>1</sup> Number of models with violations

### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)

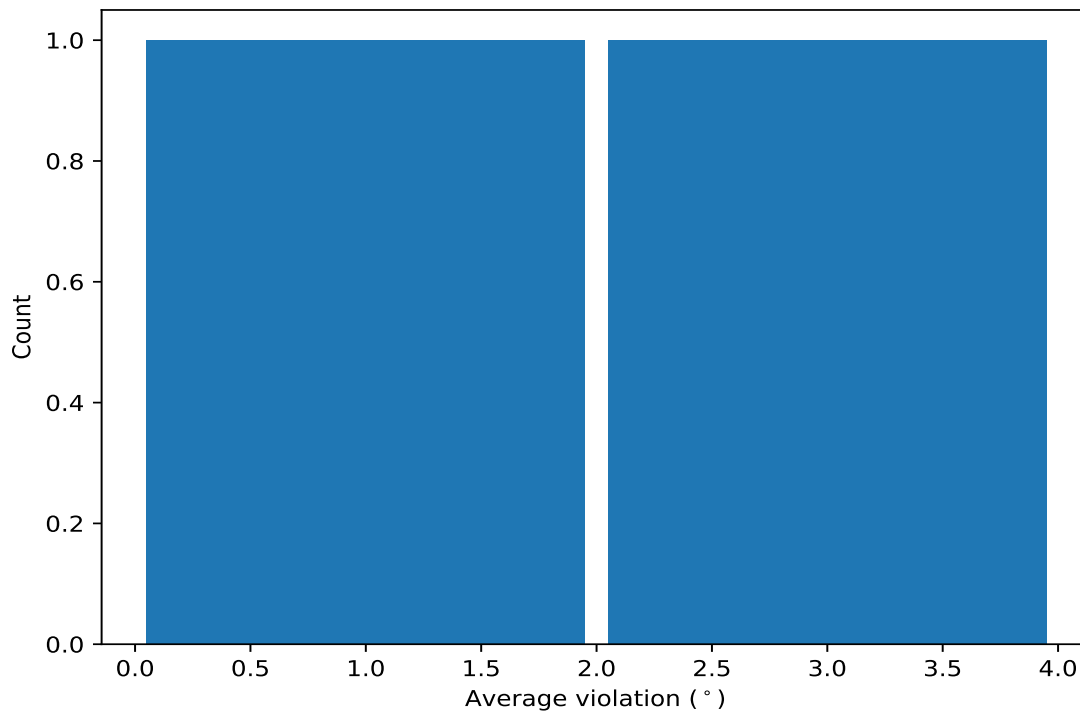


## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

### 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.

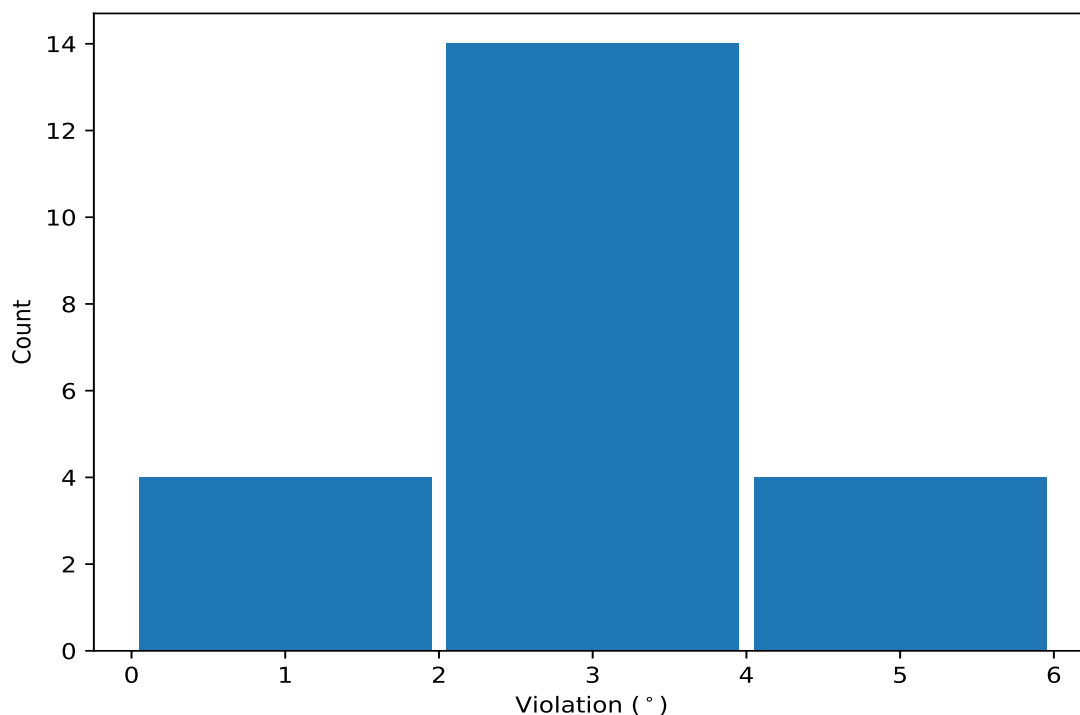
| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|--------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,51) | 1:27:A:CYS:N | 1:27:A:CYS:CA | 1:27:A:CYS:C  | 1:28:A:LYS:N | 19                  | 3.19 | 0.81            | 3.22   |
| (1,26) | 1:14:A:ASN:C | 1:15:A:ILE:N  | 1:15:A:ILE:CA | 1:15:A:ILE:C | 2                   | 1.11 | 0.02            | 1.11   |

<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 (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,51)  | 1:27:A:CYS:N | 1:27:A:CYS:CA | 1:27:A:CYS:C  | 1:28:A:LYS:N | 4        | 4.42          |
| (1,51)  | 1:27:A:CYS:N | 1:27:A:CYS:CA | 1:27:A:CYS:C  | 1:28:A:LYS:N | 15       | 4.39          |
| (1,51)  | 1:27:A:CYS:N | 1:27:A:CYS:CA | 1:27:A:CYS:C  | 1:28:A:LYS:N | 11       | 4.31          |
| (1,51)  | 1:27:A:CYS:N | 1:27:A:CYS:CA | 1:27:A:CYS:C  | 1:28:A:LYS:N | 14       | 4.12          |
| (1,51)  | 1:27:A:CYS:N | 1:27:A:CYS:CA | 1:27:A:CYS:C  | 1:28:A:LYS:N | 5        | 3.62          |
| (1,51)  | 1:27:A:CYS:N | 1:27:A:CYS:CA | 1:27:A:CYS:C  | 1:28:A:LYS:N | 13       | 3.61          |
| (1,51)  | 1:27:A:CYS:N | 1:27:A:CYS:CA | 1:27:A:CYS:C  | 1:28:A:LYS:N | 1        | 3.56          |
| (1,51)  | 1:27:A:CYS:N | 1:27:A:CYS:CA | 1:27:A:CYS:C  | 1:28:A:LYS:N | 12       | 3.34          |
| (1,51)  | 1:27:A:CYS:N | 1:27:A:CYS:CA | 1:27:A:CYS:C  | 1:28:A:LYS:N | 17       | 3.23          |
| (1,51)  | 1:27:A:CYS:N | 1:27:A:CYS:CA | 1:27:A:CYS:C  | 1:28:A:LYS:N | 2        | 3.22          |
| (1,51)  | 1:27:A:CYS:N | 1:27:A:CYS:CA | 1:27:A:CYS:C  | 1:28:A:LYS:N | 19       | 3.13          |
| (1,51)  | 1:27:A:CYS:N | 1:27:A:CYS:CA | 1:27:A:CYS:C  | 1:28:A:LYS:N | 10       | 3.09          |
| (1,51)  | 1:27:A:CYS:N | 1:27:A:CYS:CA | 1:27:A:CYS:C  | 1:28:A:LYS:N | 18       | 3.05          |
| (1,51)  | 1:27:A:CYS:N | 1:27:A:CYS:CA | 1:27:A:CYS:C  | 1:28:A:LYS:N | 7        | 2.92          |
| (1,51)  | 1:27:A:CYS:N | 1:27:A:CYS:CA | 1:27:A:CYS:C  | 1:28:A:LYS:N | 16       | 2.4           |
| (1,51)  | 1:27:A:CYS:N | 1:27:A:CYS:CA | 1:27:A:CYS:C  | 1:28:A:LYS:N | 9        | 2.36          |
| (1,51)  | 1:27:A:CYS:N | 1:27:A:CYS:CA | 1:27:A:CYS:C  | 1:28:A:LYS:N | 8        | 2.28          |
| (1,51)  | 1:27:A:CYS:N | 1:27:A:CYS:CA | 1:27:A:CYS:C  | 1:28:A:LYS:N | 6        | 2.12          |
| (1,103) | 1:56:A:ASP:N | 1:56:A:ASP:CA | 1:56:A:ASP:C  | 1:57:A:LYS:N | 4        | 1.39          |
| (1,51)  | 1:27:A:CYS:N | 1:27:A:CYS:CA | 1:27:A:CYS:C  | 1:28:A:LYS:N | 20       | 1.35          |
| (1,26)  | 1:14:A:ASN:C | 1:15:A:ILE:N  | 1:15:A:ILE:CA | 1:15:A:ILE:C | 19       | 1.13          |
| (1,26)  | 1:14:A:ASN:C | 1:15:A:ILE:N  | 1:15:A:ILE:CA | 1:15:A:ILE:C | 2        | 1.09          |