



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 05:33 AM UTC

PDB ID : 2LJX / pdb\_00002ljx  
BMRB ID : 17967  
Title : Structure of the monomeric N-terminal domain of HPV16 E6 oncoprotein  
Authors : Zanier, K.; Muhamed Sidi, A.; Boulade-Ladame, C.; Rybin, V.; Chappelle, A.;  
Atkinson, A.; Kieffer, B.; Trave, G.  
Deposited on : 2011-09-30

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

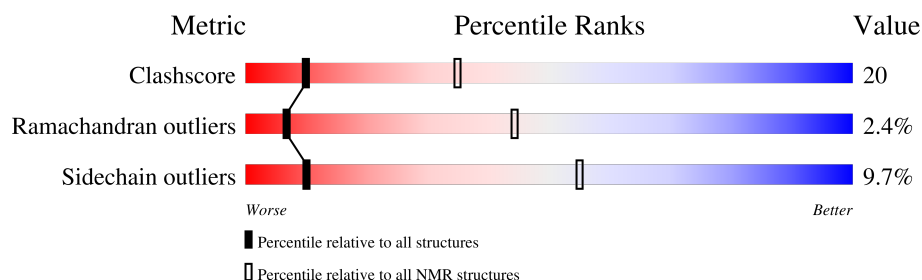
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 78%.

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     | 84     |                  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 17 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues |                       |                   |              |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:9-A:65 (57)         | 0.34              | 17           |

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 4 clusters and 4 single-model clusters were found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1374 atoms, of which 682 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein E6.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 82       | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1373  | 438 | 682 | 122 | 124 | 7 |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | -1      | GLY      | -      | expression tag      | UNP P03126 |
| A     | 47      | ARG      | PHE    | engineered mutation | UNP P03126 |
| A     | 80      | SER      | CYS    | engineered mutation | UNP P03126 |

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

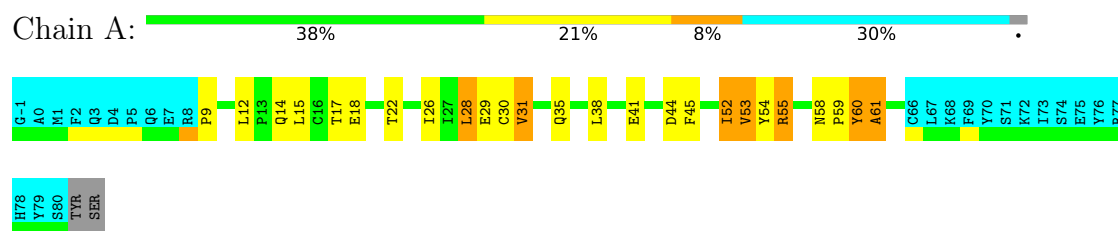
| Mol | Chain | Residues | Atoms |    |
|-----|-------|----------|-------|----|
| 2   | A     | 1        | Total | Zn |
|     |       |          | 1     | 1  |

## 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: Protein E6

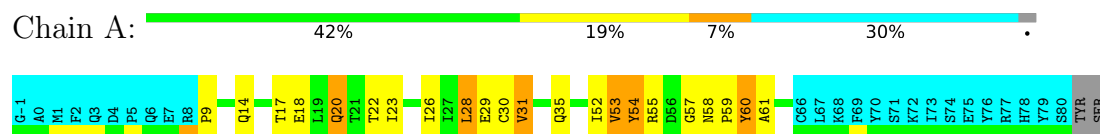


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

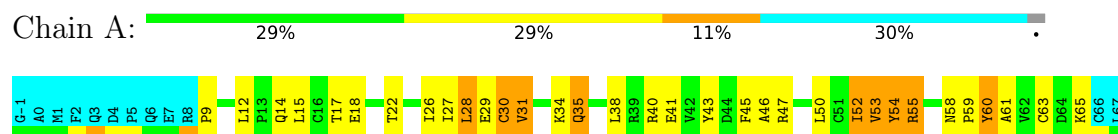
#### 4.2.1 Score per residue for model 1

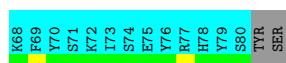
- Molecule 1: Protein E6



#### 4.2.2 Score per residue for model 2

- Molecule 1: Protein E6

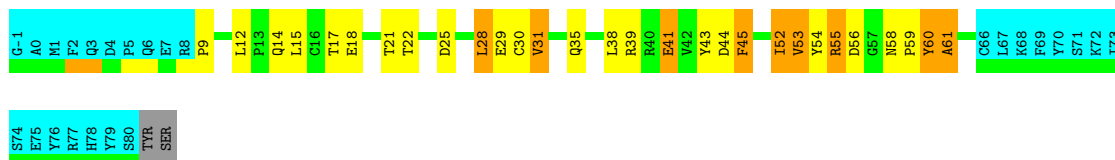




### 4.2.3 Score per residue for model 3

- Molecule 1: Protein E6

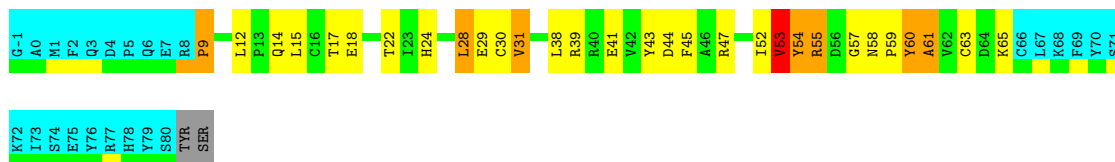
Chain A: 33% 24% 11% 30% .



### 4.2.4 Score per residue for model 4

- Molecule 1: Protein E6

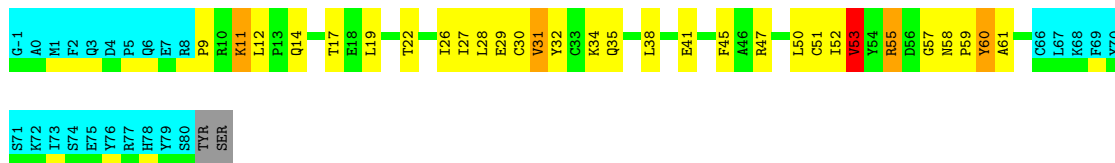
Chain A: 32% 26% 8% . 30% .



### 4.2.5 Score per residue for model 5

- Molecule 1: Protein E6

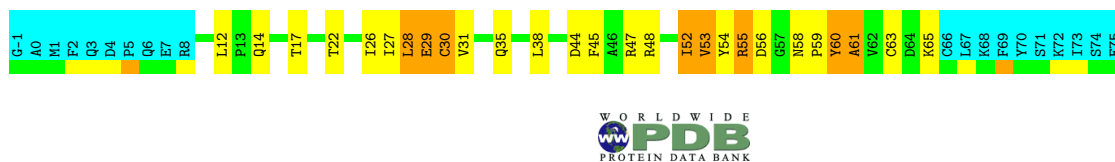
Chain A: 32% 30% 5% . 30% .

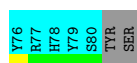


### 4.2.6 Score per residue for model 6

- Molecule 1: Protein E6

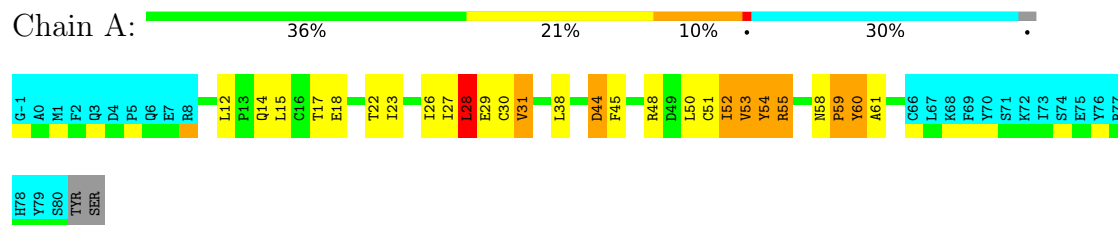
Chain A: 36% 23% 10% 30% .





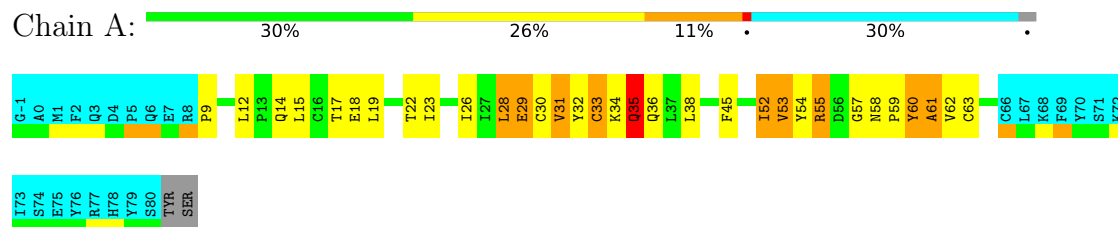
#### 4.2.7 Score per residue for model 7

- Molecule 1: Protein E6



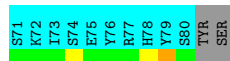
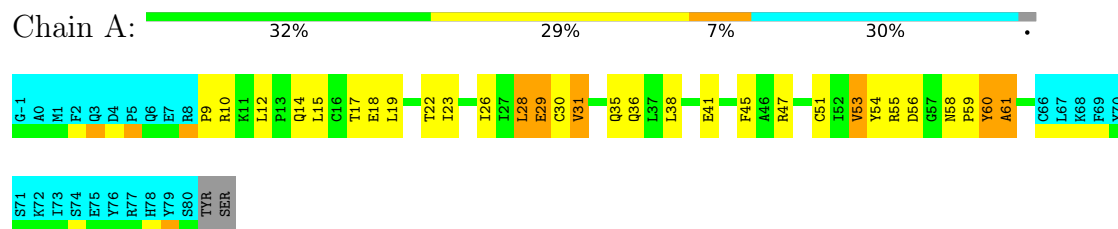
#### 4.2.8 Score per residue for model 8

- Molecule 1: Protein E6



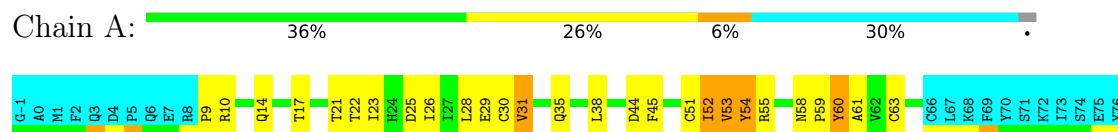
#### 4.2.9 Score per residue for model 9

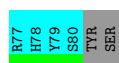
- Molecule 1: Protein E6



#### 4.2.10 Score per residue for model 10

- Molecule 1: Protein E6

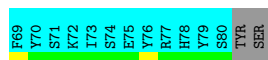
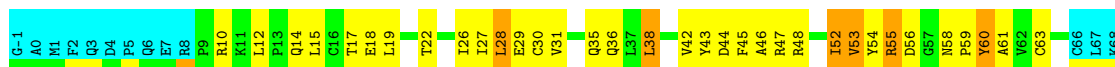




#### 4.2.11 Score per residue for model 11

- Molecule 1: Protein E6

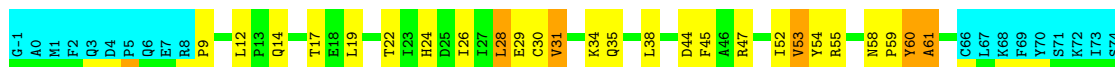
Chain A: 27% 33% 7% 30% .



#### 4.2.12 Score per residue for model 12

- Molecule 1: Protein E6

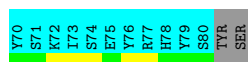
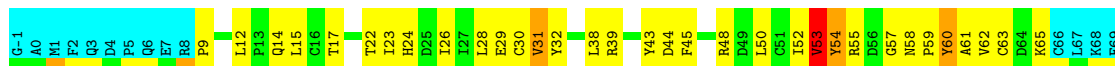
Chain A: 37% 25% 6% 30% .



#### 4.2.13 Score per residue for model 13

- Molecule 1: Protein E6

Chain A: 29% 35% 30% .



#### 4.2.14 Score per residue for model 14

- Molecule 1: Protein E6

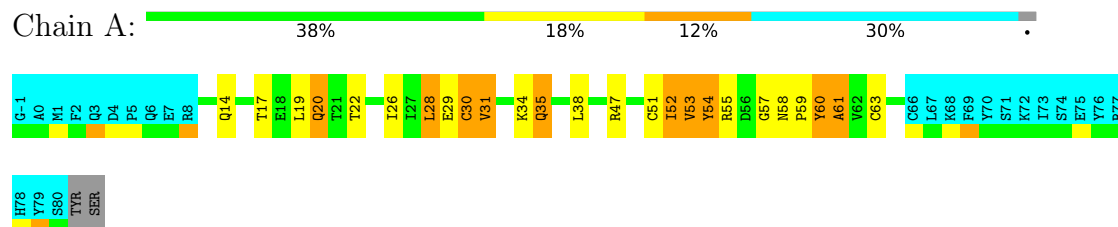
Chain A: 33% 29% 6% 30% .





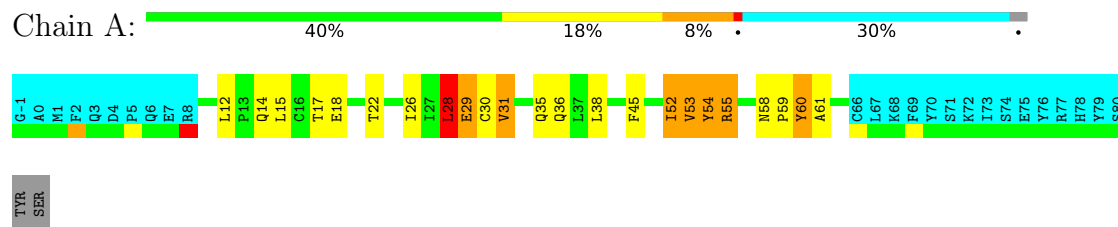
#### 4.2.15 Score per residue for model 15

- Molecule 1: Protein E6



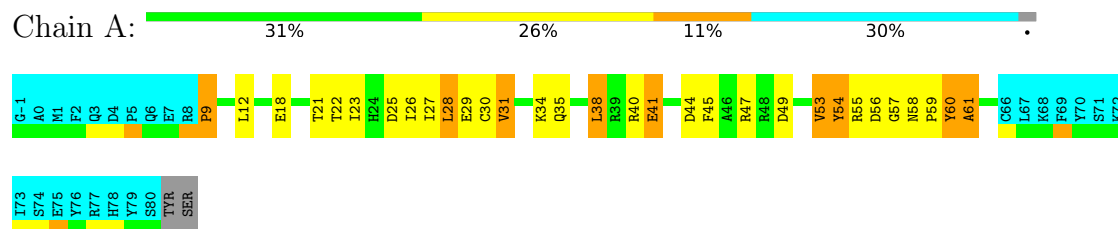
#### 4.2.16 Score per residue for model 16

- Molecule 1: Protein E6



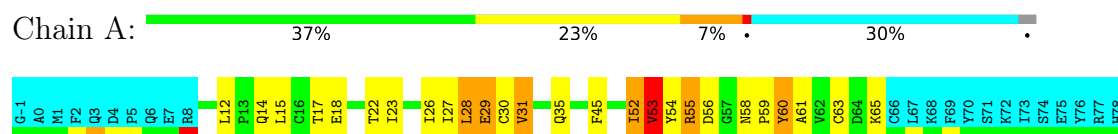
#### 4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: Protein E6



#### 4.2.18 Score per residue for model 18

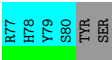
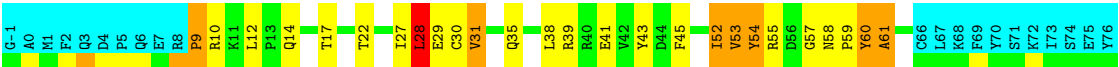
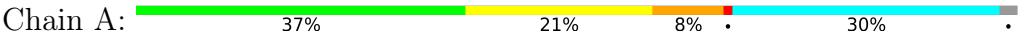
- Molecule 1: Protein E6





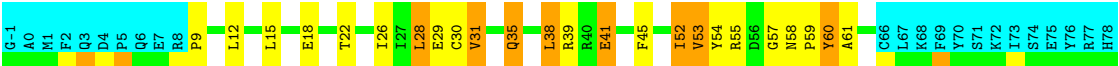
4.2.19 Score per residue for model 19

- Molecule 1: Protein E6



4.2.20 Score per residue for model 20

- Molecule 1: Protein E6



## 5 Refinement protocol and experimental data overview

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

Of the 100 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    | structure solution |         |
| X-PLOR NIH    | refinement         |         |

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                       | 901            |
| Number of shifts mapped to atoms             | 901            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 78%            |

## 6 Model quality i

### 6.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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     | 1.87±0.05    | 14±2/484 ( 3.0± 0.5%) | 1.25±0.03   | 2±1/655 ( 0.3± 0.2%) |
| All | All   | 1.87         | 290/9680 ( 3.0%)      | 1.25        | 43/13100 ( 0.3%)     |

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   | 0.2±0.4   |
| All | All   | 0         | 4         |

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     | 59  | PRO  | C-O   | 13.28  | 1.36        | 1.23     | 9      | 20    |
| 1   | A     | 60  | TYR  | N-CA  | -11.61 | 1.31        | 1.45     | 4      | 20    |
| 1   | A     | 61  | ALA  | N-CA  | -9.08  | 1.35        | 1.45     | 1      | 20    |
| 1   | A     | 60  | TYR  | C-N   | -8.64  | 1.20        | 1.33     | 3      | 20    |
| 1   | A     | 30  | CYS  | C-N   | -8.13  | 1.23        | 1.33     | 14     | 20    |
| 1   | A     | 28  | LEU  | CA-C  | -7.60  | 1.43        | 1.52     | 16     | 11    |
| 1   | A     | 53  | VAL  | N-CA  | -7.18  | 1.37        | 1.46     | 10     | 20    |
| 1   | A     | 35  | GLN  | N-CA  | -7.11  | 1.37        | 1.46     | 17     | 11    |
| 1   | A     | 30  | CYS  | N-CA  | -7.02  | 1.37        | 1.46     | 9      | 12    |
| 1   | A     | 36  | GLN  | N-CA  | -6.65  | 1.38        | 1.46     | 16     | 4     |
| 1   | A     | 28  | LEU  | N-CA  | -6.52  | 1.38        | 1.46     | 2      | 16    |
| 1   | A     | 59  | PRO  | C-N   | -6.49  | 1.24        | 1.33     | 19     | 18    |
| 1   | A     | 35  | GLN  | C-N   | -6.47  | 1.24        | 1.33     | 9      | 3     |
| 1   | A     | 52  | ILE  | C-N   | -6.27  | 1.24        | 1.33     | 10     | 16    |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|-------|-------------|----------|--------|-------|
|     |       |     |      |       |       |             |          | Worst  | Total |
| 1   | A     | 54  | TYR  | CA-C  | -6.05 | 1.45        | 1.52     | 13     | 10    |
| 1   | A     | 61  | ALA  | C-N   | -6.04 | 1.25        | 1.33     | 9      | 15    |
| 1   | A     | 54  | TYR  | N-CA  | -6.03 | 1.39        | 1.46     | 10     | 6     |
| 1   | A     | 27  | ILE  | N-CA  | -5.94 | 1.39        | 1.46     | 2      | 8     |
| 1   | A     | 60  | TYR  | CA-C  | -5.77 | 1.45        | 1.52     | 8      | 11    |
| 1   | A     | 53  | VAL  | C-N   | -5.73 | 1.25        | 1.33     | 7      | 10    |
| 1   | A     | 35  | GLN  | CA-C  | -5.67 | 1.45        | 1.52     | 16     | 1     |
| 1   | A     | 27  | ILE  | CA-C  | -5.60 | 1.47        | 1.53     | 2      | 1     |
| 1   | A     | 52  | ILE  | CA-C  | -5.57 | 1.46        | 1.52     | 7      | 3     |
| 1   | A     | 44  | ASP  | C-N   | -5.45 | 1.26        | 1.33     | 12     | 6     |
| 1   | A     | 29  | GLU  | CA-C  | -5.44 | 1.45        | 1.53     | 8      | 3     |
| 1   | A     | 38  | LEU  | N-CA  | -5.38 | 1.39        | 1.46     | 5      | 2     |
| 1   | A     | 45  | PHE  | N-CA  | -5.31 | 1.39        | 1.46     | 3      | 2     |
| 1   | A     | 59  | PRO  | CA-C  | 5.06  | 1.57        | 1.52     | 7      | 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     | 34  | LYS  | N-CA-C  | 7.12  | 119.25      | 110.91   | 8      | 1     |
| 1   | A     | 28  | LEU  | CA-C-N  | -5.96 | 112.25      | 123.27   | 9      | 14    |
| 1   | A     | 28  | LEU  | C-N-CA  | -5.96 | 112.25      | 123.27   | 9      | 14    |
| 1   | A     | 59  | PRO  | CA-C-O  | 5.56  | 127.75      | 120.85   | 9      | 12    |
| 1   | A     | 59  | PRO  | N-CA-C  | 5.16  | 118.68      | 110.21   | 11     | 1     |
| 1   | A     | 29  | GLU  | N-CA-CB | 5.01  | 118.21      | 110.60   | 6      | 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     | 48  | ARG  | Sidechain | 2              |
| 1   | A     | 39  | ARG  | Sidechain | 1              |
| 1   | A     | 10  | ARG  | Sidechain | 1              |

## 6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 475   | 479      | 479      | 19±3    |
| All | All   | 9520  | 9580     | 9580     | 373     |

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 20.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:29:GLU:HG3  | 1:A:60:TYR:CD2  | 0.73     | 2.18        | 16     | 1     |
| 1:A:29:GLU:HG3  | 1:A:60:TYR:CD1  | 0.68     | 2.24        | 5      | 18    |
| 1:A:29:GLU:HG2  | 1:A:60:TYR:CD1  | 0.68     | 2.24        | 6      | 1     |
| 1:A:31:VAL:O    | 1:A:55:ARG:HG3  | 0.61     | 1.95        | 6      | 19    |
| 1:A:29:GLU:O    | 1:A:60:TYR:HB3  | 0.61     | 1.96        | 9      | 20    |
| 1:A:14:GLN:O    | 1:A:17:THR:HB   | 0.60     | 1.97        | 4      | 18    |
| 1:A:33:CYS:HB2  | 1:A:35:GLN:NE2  | 0.59     | 2.13        | 8      | 1     |
| 1:A:33:CYS:HB2  | 1:A:35:GLN:HE22 | 0.58     | 1.59        | 8      | 1     |
| 1:A:63:CYS:SG   | 1:A:65:LYS:HB2  | 0.58     | 2.39        | 13     | 4     |
| 1:A:58:ASN:HB2  | 1:A:60:TYR:CE1  | 0.58     | 2.34        | 16     | 1     |
| 1:A:31:VAL:HB   | 1:A:60:TYR:HB2  | 0.57     | 1.76        | 7      | 19    |
| 1:A:31:VAL:HG11 | 1:A:53:VAL:CG2  | 0.56     | 2.31        | 8      | 20    |
| 1:A:31:VAL:HG23 | 1:A:55:ARG:CB   | 0.56     | 2.31        | 14     | 20    |
| 1:A:58:ASN:HB2  | 1:A:60:TYR:CZ   | 0.55     | 2.36        | 5      | 19    |
| 1:A:44:ASP:HB3  | 1:A:48:ARG:CZ   | 0.55     | 2.31        | 13     | 1     |
| 1:A:63:CYS:SG   | 1:A:65:LYS:HE3  | 0.54     | 2.42        | 6      | 1     |
| 1:A:26:ILE:HD11 | 1:A:28:LEU:HD13 | 0.54     | 1.79        | 8      | 11    |
| 1:A:58:ASN:HB2  | 1:A:60:TYR:CE2  | 0.53     | 2.39        | 7      | 17    |
| 1:A:31:VAL:HG23 | 1:A:55:ARG:HB2  | 0.53     | 1.81        | 14     | 12    |
| 1:A:54:TYR:HA   | 1:A:58:ASN:O    | 0.52     | 2.04        | 1      | 15    |
| 1:A:12:LEU:HD22 | 1:A:45:PHE:HB3  | 0.52     | 1.82        | 5      | 17    |
| 1:A:19:LEU:HD22 | 1:A:26:ILE:HG13 | 0.51     | 1.80        | 8      | 6     |
| 1:A:31:VAL:HG23 | 1:A:55:ARG:CG   | 0.51     | 2.36        | 8      | 4     |
| 1:A:52:ILE:HG23 | 1:A:60:TYR:O    | 0.50     | 2.07        | 16     | 13    |
| 1:A:31:VAL:HG22 | 1:A:32:TYR:CE1  | 0.49     | 2.43        | 5      | 2     |
| 1:A:9:PRO:HD3   | 1:A:18:GLU:OE2  | 0.49     | 2.06        | 17     | 2     |
| 1:A:12:LEU:HD23 | 1:A:46:ALA:HB2  | 0.49     | 1.84        | 11     | 2     |
| 1:A:50:LEU:N    | 1:A:50:LEU:HD12 | 0.49     | 2.22        | 13     | 3     |
| 1:A:15:LEU:O    | 1:A:18:GLU:HB2  | 0.49     | 2.07        | 9      | 9     |
| 1:A:9:PRO:O     | 1:A:10:ARG:HD2  | 0.49     | 2.08        | 9      | 2     |
| 1:A:28:LEU:HD23 | 1:A:61:ALA:HB2  | 0.49     | 1.84        | 12     | 10    |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:48:ARG:HB2  | 1:A:50:LEU:CD1  | 0.48     | 2.38        | 13     | 2     |
| 1:A:29:GLU:CG   | 1:A:60:TYR:CD1  | 0.48     | 2.95        | 5      | 18    |
| 1:A:31:VAL:HG11 | 1:A:53:VAL:HG21 | 0.47     | 1.86        | 12     | 8     |
| 1:A:38:LEU:HB3  | 1:A:41:GLU:OE1  | 0.47     | 2.09        | 20     | 2     |
| 1:A:41:GLU:HA   | 1:A:44:ASP:OD2  | 0.47     | 2.10        | 4      | 2     |
| 1:A:43:TYR:O    | 1:A:47:ARG:HD3  | 0.46     | 2.11        | 2      | 3     |
| 1:A:29:GLU:HG3  | 1:A:60:TYR:CE1  | 0.46     | 2.46        | 4      | 1     |
| 1:A:9:PRO:HD2   | 1:A:15:LEU:HD13 | 0.46     | 1.88        | 20     | 3     |
| 1:A:11:LYS:HD3  | 1:A:14:GLN:NE2  | 0.46     | 2.26        | 5      | 1     |
| 1:A:21:THR:OG1  | 1:A:25:ASP:HB3  | 0.45     | 2.12        | 3      | 4     |
| 1:A:30:CYS:HB2  | 1:A:63:CYS:HB3  | 0.45     | 1.87        | 15     | 3     |
| 1:A:29:GLU:CG   | 1:A:60:TYR:HD1  | 0.44     | 2.25        | 7      | 2     |
| 1:A:31:VAL:HG23 | 1:A:55:ARG:HG2  | 0.44     | 1.88        | 18     | 3     |
| 1:A:10:ARG:HD2  | 1:A:52:ILE:O    | 0.44     | 2.11        | 11     | 1     |
| 1:A:23:ILE:HA   | 1:A:26:ILE:HG22 | 0.44     | 1.88        | 9      | 8     |
| 1:A:20:GLN:HE21 | 1:A:20:GLN:HA   | 0.44     | 1.73        | 1      | 1     |
| 1:A:40:ARG:HB2  | 1:A:41:GLU:OE1  | 0.44     | 2.12        | 17     | 1     |
| 1:A:38:LEU:O    | 1:A:42:VAL:HG23 | 0.44     | 2.13        | 11     | 1     |
| 1:A:52:ILE:HG22 | 1:A:54:TYR:CE1  | 0.43     | 2.49        | 14     | 2     |
| 1:A:23:ILE:HA   | 1:A:26:ILE:CG2  | 0.43     | 2.44        | 9      | 3     |
| 1:A:39:ARG:HG2  | 1:A:43:TYR:CE2  | 0.42     | 2.49        | 13     | 3     |
| 1:A:29:GLU:HG3  | 1:A:60:TYR:CE2  | 0.42     | 2.49        | 16     | 1     |
| 1:A:31:VAL:HG22 | 1:A:32:TYR:CD1  | 0.42     | 2.50        | 8      | 2     |
| 1:A:44:ASP:HB3  | 1:A:48:ARG:NH2  | 0.42     | 2.29        | 7      | 1     |
| 1:A:45:PHE:HA   | 1:A:50:LEU:HD13 | 0.41     | 1.92        | 5      | 1     |
| 1:A:40:ARG:HB2  | 1:A:41:GLU:OE2  | 0.41     | 2.16        | 2      | 1     |
| 1:A:28:LEU:HD12 | 1:A:28:LEU:HA   | 0.41     | 1.64        | 16     | 1     |
| 1:A:39:ARG:HG3  | 1:A:43:TYR:CE2  | 0.41     | 2.51        | 19     | 1     |
| 1:A:29:GLU:HG3  | 1:A:60:TYR:HD1  | 0.41     | 1.73        | 4      | 1     |
| 1:A:20:GLN:HA   | 1:A:20:GLN:HE21 | 0.40     | 1.76        | 15     | 1     |
| 1:A:41:GLU:O    | 1:A:44:ASP:HB2  | 0.40     | 2.16        | 3      | 1     |
| 1:A:34:LYS:HD2  | 1:A:34:LYS:N    | 0.40     | 2.32        | 17     | 1     |

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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

| Mol | Chain | Analysed        | Favoured     | Allowed     | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|-------------|------------|-------------|----|
| 1   | A     | 57/84 (68%)     | 50±1 (88±2%) | 6±2 (10±3%) | 1±1 (2±1%) | 7           | 44 |
| All | All   | 1140/1680 (68%) | 999 (88%)    | 114 (10%)   | 27 (2%)    | 7           | 44 |

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 9   | PRO  | 10             |
| 1   | A     | 57  | GLY  | 10             |
| 1   | A     | 56  | ASP  | 6              |
| 1   | A     | 51  | CYS  | 1              |

### 6.3.2 Protein sidechains ⓘ

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

| Mol | Chain | Analysed        | Rotameric    | Outliers    | Percentiles |    |
|-----|-------|-----------------|--------------|-------------|-------------|----|
| 1   | A     | 54/79 (68%)     | 49±1 (90±2%) | 5±1 (10±2%) | 10          | 55 |
| All | All   | 1080/1580 (68%) | 975 (90%)    | 105 (10%)   | 10          | 55 |

All 17 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     | 22  | THR  | 20             |
| 1   | A     | 31  | VAL  | 18             |
| 1   | A     | 38  | LEU  | 16             |
| 1   | A     | 55  | ARG  | 10             |
| 1   | A     | 35  | GLN  | 7              |
| 1   | A     | 41  | GLU  | 6              |
| 1   | A     | 47  | ARG  | 6              |
| 1   | A     | 34  | LYS  | 4              |
| 1   | A     | 53  | VAL  | 4              |
| 1   | A     | 24  | HIS  | 3              |
| 1   | A     | 28  | LEU  | 3              |
| 1   | A     | 18  | GLU  | 2              |
| 1   | A     | 20  | GLN  | 2              |
| 1   | A     | 11  | LYS  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 33  | CYS  | 1              |
| 1   | A     | 29  | GLU  | 1              |
| 1   | A     | 39  | ARG  | 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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

## 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 78% for the well-defined parts and 75% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *E6N*

#### 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                  | 901 |
| Number of shifts mapped to atoms        | 901 |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 0   |
| Number of shifts with mapping warnings  | 0   |
| Number of shift outliers (ShiftChecker) | 1   |

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

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 82       | $-0.47 \pm 0.43$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 80       | $0.10 \pm 0.21$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 0        | —                               | None (insufficient data)   |
| $^{15}\text{N}$        | 76       | $-1.52 \pm 0.67$                | 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 78%, i.e. 653 atoms were assigned a chemical shift out of a possible 837. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$   | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 223/280 (80%) | 112/112 (100%) | 57/114 (50%)    | 54/54 (100%)    |
| Sidechain | 417/504 (83%) | 278/325 (86%)  | 134/153 (88%)   | 5/26 (19%)      |

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|          | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|---------------|----------------|-----------------|-----------------|
| Aromatic | 13/53 (25%)   | 13/25 (52%)    | 0/27 (0%)       | 0/1 (0%)        |
| Overall  | 653/837 (78%) | 403/462 (87%)  | 191/294 (65%)   | 59/81 (73%)     |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 75%, i.e. 901 atoms were assigned a chemical shift out of a possible 1194. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|----------------|----------------|-----------------|-----------------|
| Backbone  | 317/404 (78%)  | 159/162 (98%)  | 82/164 (50%)    | 76/78 (97%)     |
| Sidechain | 557/683 (82%)  | 368/439 (84%)  | 182/208 (88%)   | 7/36 (19%)      |
| Aromatic  | 27/107 (25%)   | 27/51 (53%)    | 0/54 (0%)       | 0/2 (0%)        |
| Overall   | 901/1194 (75%) | 554/652 (85%)  | 264/426 (62%)   | 83/116 (72%)    |

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

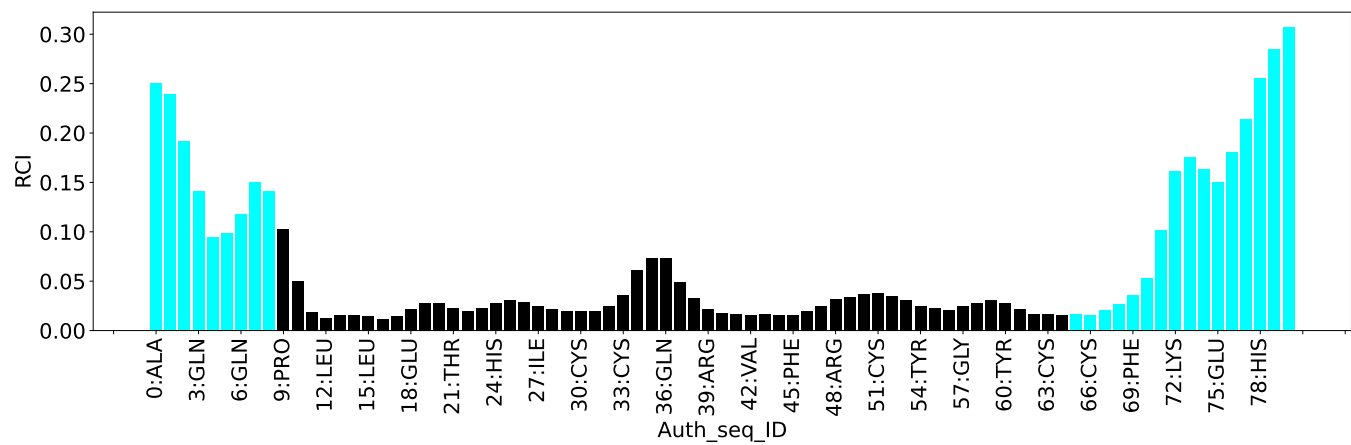
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 37  | LEU  | CG   | 32.63      | 21.37 – 32.19       | 5.4     |

#### 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                                | 1256  |
| Intra-residue ( $ i-j =0$ )                              | 433   |
| Sequential ( $ i-j =1$ )                                 | 310   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 191   |
| Long range ( $ i-j \geq 5$ )                             | 322   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 87    |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 15.8  |
| Number of long range restraints per residue <sup>1</sup> | 3.8   |

<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)  | 53.5                                   | 0.2     |
| 0.2-0.5 (Medium) | 12.6                                   | 0.38    |
| >0.5 (Large)     | 1.0                                    | 3.0     |

### 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)   | 5.8                                    | 4.88    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

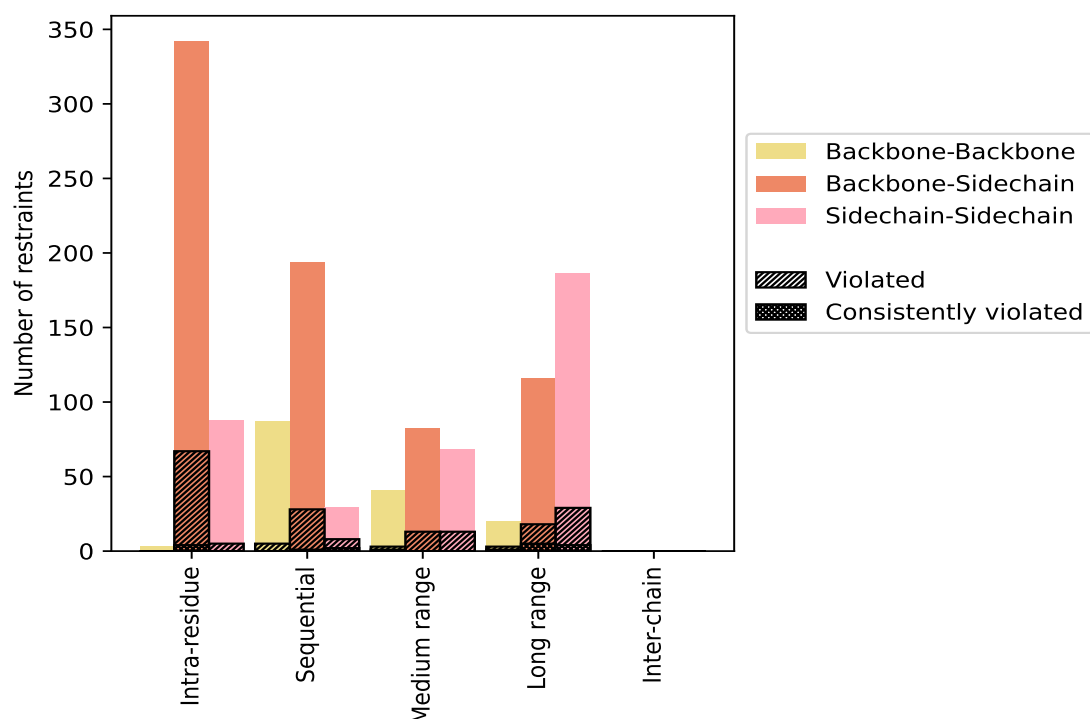
### 9.1 Summary of distance violations ⓘ

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>433</b>  | <b>34.5</b>    | <b>72</b>             | <b>16.6</b>    | <b>5.7</b>     | <b>4</b>                           | <b>0.9</b>     | <b>0.3</b>     |
| Backbone-Backbone                                                           | 3           | 0.2            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 342         | 27.2           | 67                    | 19.6           | 5.3            | 4                                  | 1.2            | 0.3            |
| Sidechain-Sidechain                                                         | 88          | 7.0            | 5                     | 5.7            | 0.4            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>310</b>  | <b>24.7</b>    | <b>41</b>             | <b>13.2</b>    | <b>3.3</b>     | <b>3</b>                           | <b>1.0</b>     | <b>0.2</b>     |
| Backbone-Backbone                                                           | 87          | 6.9            | 5                     | 5.7            | 0.4            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 194         | 15.4           | 28                    | 14.4           | 2.2            | 1                                  | 0.5            | 0.1            |
| Sidechain-Sidechain                                                         | 29          | 2.3            | 8                     | 27.6           | 0.6            | 2                                  | 6.9            | 0.2            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>191</b>  | <b>15.2</b>    | <b>29</b>             | <b>15.2</b>    | <b>2.3</b>     | <b>1</b>                           | <b>0.5</b>     | <b>0.1</b>     |
| Backbone-Backbone                                                           | 41          | 3.3            | 3                     | 7.3            | 0.2            | 1                                  | 2.4            | 0.1            |
| Backbone-Sidechain                                                          | 82          | 6.5            | 13                    | 15.9           | 1.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 68          | 5.4            | 13                    | 19.1           | 1.0            | 0                                  | 0.0            | 0.0            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>322</b>  | <b>25.6</b>    | <b>50</b>             | <b>15.5</b>    | <b>4.0</b>     | <b>10</b>                          | <b>3.1</b>     | <b>0.8</b>     |
| Backbone-Backbone                                                           | 20          | 1.6            | 3                     | 15.0           | 0.2            | 1                                  | 5.0            | 0.1            |
| Backbone-Sidechain                                                          | 116         | 9.2            | 18                    | 15.5           | 1.4            | 5                                  | 4.3            | 0.4            |
| Sidechain-Sidechain                                                         | 186         | 14.8           | 29                    | 15.6           | 2.3            | 4                                  | 2.2            | 0.3            |
| <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>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>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>1256</b> | <b>100.0</b>   | <b>192</b>            | <b>15.3</b>    | <b>15.3</b>    | <b>18</b>                          | <b>1.4</b>     | <b>1.4</b>     |
| Backbone-Backbone                                                           | 151         | 12.0           | 11                    | 7.3            | 0.9            | 2                                  | 1.3            | 0.2            |
| Backbone-Sidechain                                                          | 734         | 58.4           | 126                   | 17.2           | 10.0           | 10                                 | 1.4            | 0.8            |
| Sidechain-Sidechain                                                         | 371         | 29.5           | 55                    | 14.8           | 4.4            | 6                                  | 1.6            | 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 disulfied bonds are counted in their appropriate category on the x-axis

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 27                   | 10              | 9               | 23              | 0               | 69    | 0.19     | 2.79    | 0.32                | 0.14       |
| 2        | 31                   | 13              | 10              | 25              | 0               | 79    | 0.18     | 2.37    | 0.25                | 0.14       |
| 3        | 22                   | 14              | 12              | 25              | 0               | 73    | 0.19     | 2.52    | 0.28                | 0.14       |
| 4        | 24                   | 13              | 6               | 27              | 0               | 70    | 0.2      | 2.74    | 0.31                | 0.15       |
| 5        | 23                   | 13              | 8               | 22              | 0               | 66    | 0.2      | 2.91    | 0.34                | 0.14       |
| 6        | 24                   | 6               | 9               | 26              | 0               | 65    | 0.2      | 2.64    | 0.31                | 0.15       |
| 7        | 24                   | 11              | 11              | 28              | 0               | 74    | 0.2      | 3.0     | 0.33                | 0.15       |
| 8        | 24                   | 12              | 8               | 27              | 0               | 71    | 0.2      | 2.49    | 0.28                | 0.14       |
| 9        | 24                   | 16              | 10              | 25              | 0               | 75    | 0.19     | 2.61    | 0.28                | 0.15       |
| 10       | 27                   | 11              | 8               | 26              | 0               | 72    | 0.2      | 2.8     | 0.31                | 0.16       |

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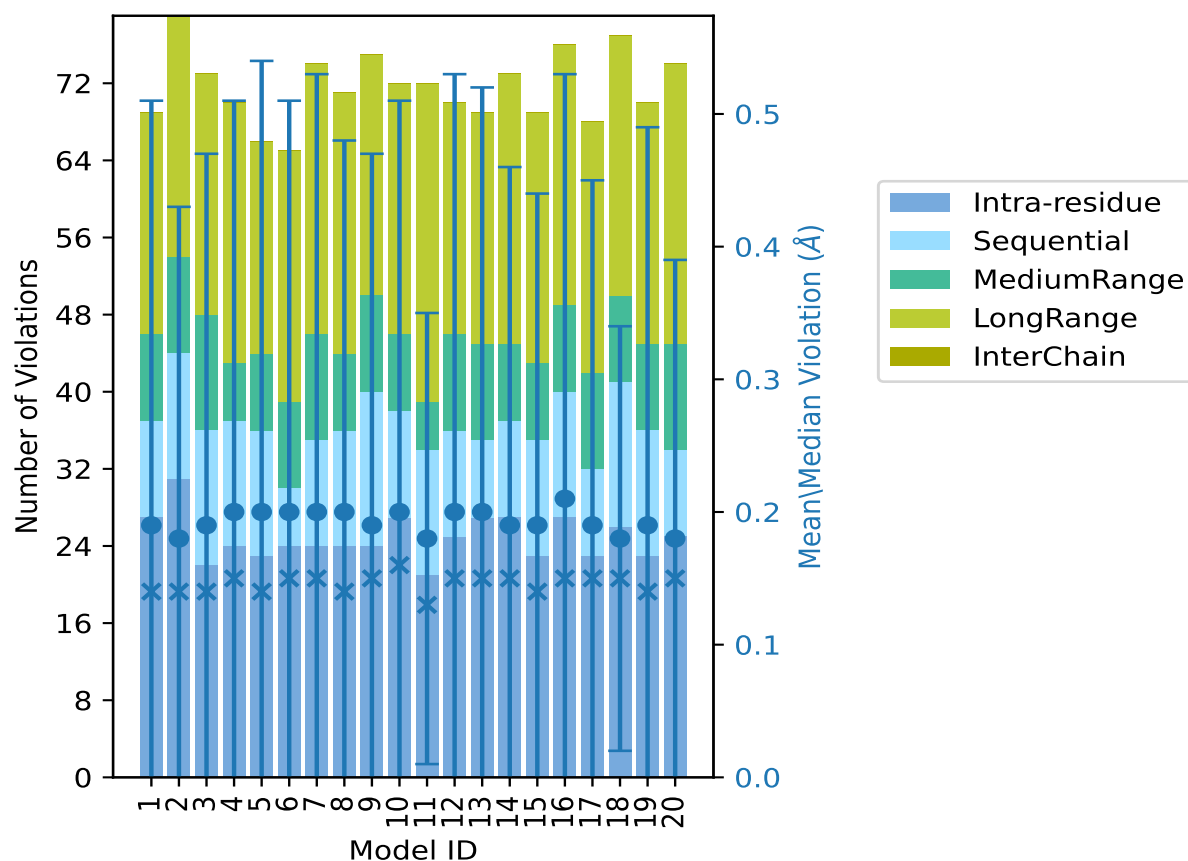
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 21                   | 13              | 5               | 33              | 0               | 72    | 0.18     | 1.52    | 0.17                | 0.13       |
| 12       | 25                   | 11              | 10              | 24              | 0               | 70    | 0.2      | 2.87    | 0.33                | 0.15       |
| 13       | 27                   | 8               | 10              | 24              | 0               | 69    | 0.2      | 2.83    | 0.32                | 0.15       |
| 14       | 27                   | 10              | 8               | 28              | 0               | 73    | 0.19     | 2.48    | 0.27                | 0.15       |
| 15       | 23                   | 12              | 8               | 26              | 0               | 69    | 0.19     | 2.23    | 0.25                | 0.14       |
| 16       | 27                   | 13              | 9               | 27              | 0               | 76    | 0.21     | 2.9     | 0.32                | 0.15       |
| 17       | 23                   | 9               | 10              | 26              | 0               | 68    | 0.19     | 2.29    | 0.26                | 0.15       |
| 18       | 26                   | 15              | 9               | 27              | 0               | 77    | 0.18     | 1.53    | 0.16                | 0.15       |
| 19       | 23                   | 13              | 9               | 25              | 0               | 70    | 0.19     | 2.63    | 0.3                 | 0.14       |
| 20       | 25                   | 9               | 11              | 29              | 0               | 74    | 0.18     | 1.97    | 0.21                | 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

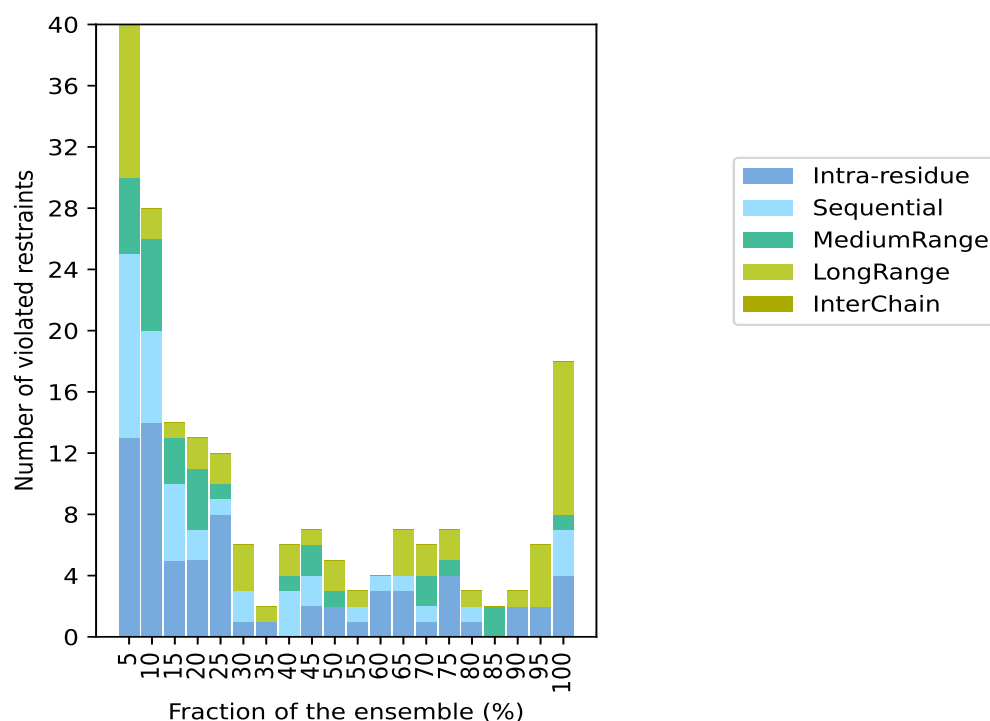
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1064(IR:361, SQ:269, MR:162, LR:272, IC:0) restraints are 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>       | %     |
| 13                            | 12              | 5               | 10              | 0               | 40    | 1                        | 5.0   |
| 14                            | 6               | 6               | 2               | 0               | 28    | 2                        | 10.0  |
| 5                             | 5               | 3               | 1               | 0               | 14    | 3                        | 15.0  |
| 5                             | 2               | 4               | 2               | 0               | 13    | 4                        | 20.0  |
| 8                             | 1               | 1               | 2               | 0               | 12    | 5                        | 25.0  |
| 1                             | 2               | 0               | 3               | 0               | 6     | 6                        | 30.0  |
| 1                             | 0               | 0               | 1               | 0               | 2     | 7                        | 35.0  |
| 0                             | 3               | 1               | 2               | 0               | 6     | 8                        | 40.0  |
| 2                             | 2               | 2               | 1               | 0               | 7     | 9                        | 45.0  |
| 2                             | 0               | 1               | 2               | 0               | 5     | 10                       | 50.0  |
| 1                             | 1               | 0               | 1               | 0               | 3     | 11                       | 55.0  |
| 3                             | 1               | 0               | 0               | 0               | 4     | 12                       | 60.0  |
| 3                             | 1               | 0               | 3               | 0               | 7     | 13                       | 65.0  |
| 1                             | 1               | 2               | 2               | 0               | 6     | 14                       | 70.0  |
| 4                             | 0               | 1               | 2               | 0               | 7     | 15                       | 75.0  |
| 1                             | 1               | 0               | 1               | 0               | 3     | 16                       | 80.0  |
| 0                             | 0               | 2               | 0               | 0               | 2     | 17                       | 85.0  |
| 2                             | 0               | 0               | 1               | 0               | 3     | 18                       | 90.0  |
| 2                             | 0               | 0               | 4               | 0               | 6     | 19                       | 95.0  |
| 4                             | 3               | 1               | 10              | 0               | 18    | 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

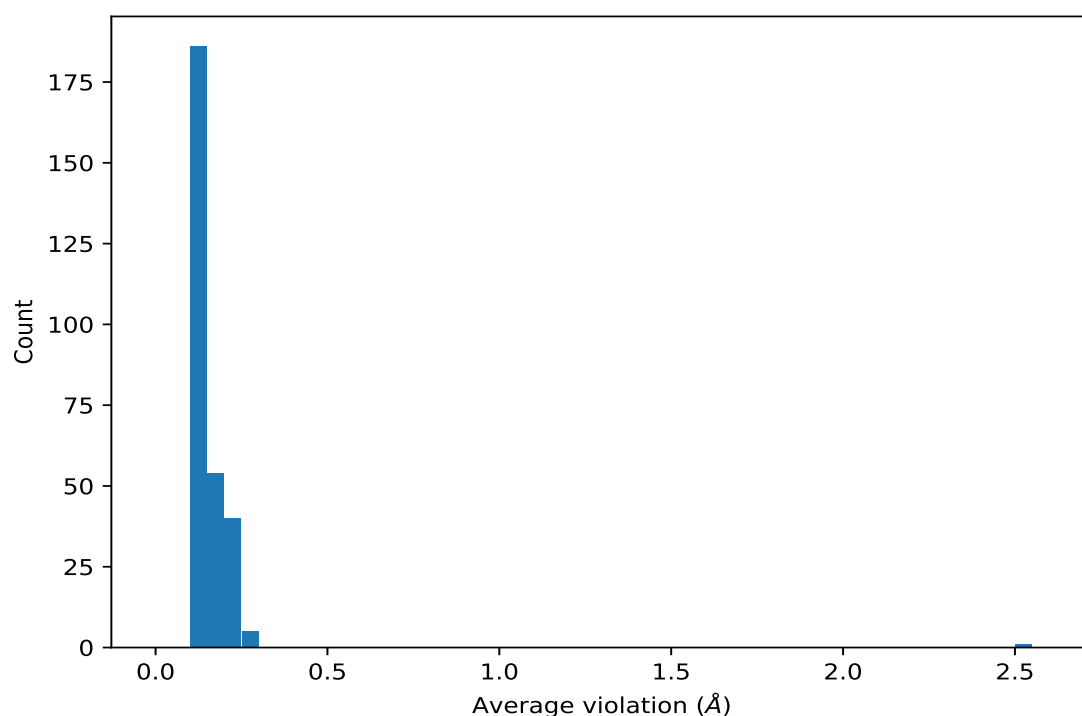
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1237) | 1:59:A:PRO:HD3  | 1:8:A:ARG:H     | 20                  | 2.51     | 0.41                | 2.62       |
| (1,1030) | 1:27:A:ILE:HA   | 1:28:A:LEU:HD11 | 20                  | 0.3      | 0.01                | 0.3        |
| (1,1030) | 1:27:A:ILE:HA   | 1:28:A:LEU:HD12 | 20                  | 0.3      | 0.01                | 0.3        |
| (1,1030) | 1:27:A:ILE:HA   | 1:28:A:LEU:HD13 | 20                  | 0.3      | 0.01                | 0.3        |
| (1,1056) | 1:31:A:VAL:HG11 | 1:55:A:ARG:HA   | 20                  | 0.24     | 0.03                | 0.24       |
| (1,1056) | 1:31:A:VAL:HG12 | 1:55:A:ARG:HA   | 20                  | 0.24     | 0.03                | 0.24       |
| (1,1056) | 1:31:A:VAL:HG13 | 1:55:A:ARG:HA   | 20                  | 0.24     | 0.03                | 0.24       |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB1  | 20                  | 0.23     | 0.02                | 0.23       |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB2  | 20                  | 0.23     | 0.02                | 0.23       |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB3  | 20                  | 0.23     | 0.02                | 0.23       |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB1  | 20                  | 0.23     | 0.02                | 0.23       |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB2  | 20                  | 0.23     | 0.02                | 0.23       |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB3  | 20                  | 0.23     | 0.02                | 0.23       |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB1  | 20                  | 0.23     | 0.02                | 0.23       |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB2  | 20                  | 0.23     | 0.02                | 0.23       |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB3  | 20                  | 0.23     | 0.02                | 0.23       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,340)  | 1:44:A:ASP:HB2  | 1:45:A:PHE:HD1  | 20                  | 0.23     | 0.04                | 0.21       |
| (1,340)  | 1:44:A:ASP:HB2  | 1:45:A:PHE:HD2  | 20                  | 0.23     | 0.04                | 0.21       |
| (1,1244) | 1:30:A:CYS:H    | 1:63:A:CYS:H    | 20                  | 0.22     | 0.03                | 0.22       |
| (1,1242) | 1:29:A:GLU:HB2  | 1:60:A:TYR:HB2  | 20                  | 0.21     | 0.03                | 0.21       |
| (1,1229) | 1:55:A:ARG:HG3  | 1:32:A:TYR:H    | 20                  | 0.2      | 0.03                | 0.21       |
| (1,649)  | 1:52:A:ILE:HA   | 1:62:A:VAL:HG21 | 20                  | 0.2      | 0.03                | 0.2        |
| (1,649)  | 1:52:A:ILE:HA   | 1:62:A:VAL:HG22 | 20                  | 0.2      | 0.03                | 0.2        |
| (1,649)  | 1:52:A:ILE:HA   | 1:62:A:VAL:HG23 | 20                  | 0.2      | 0.03                | 0.2        |
| (1,283)  | 1:23:A:ILE:HG12 | 1:24:A:HIS:HE1  | 20                  | 0.19     | 0.01                | 0.19       |
| (1,53)   | 1:37:A:LEU:H    | 1:37:A:LEU:HB3  | 20                  | 0.18     | 0.02                | 0.18       |
| (1,1253) | 1:32:A:TYR:HE1  | 1:62:A:VAL:HB   | 20                  | 0.18     | 0.02                | 0.18       |
| (1,1253) | 1:32:A:TYR:HE2  | 1:62:A:VAL:HB   | 20                  | 0.18     | 0.02                | 0.18       |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB1  | 20                  | 0.18     | 0.02                | 0.18       |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB2  | 20                  | 0.18     | 0.02                | 0.18       |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB3  | 20                  | 0.18     | 0.02                | 0.18       |
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG11 | 20                  | 0.17     | 0.03                | 0.17       |
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG12 | 20                  | 0.17     | 0.03                | 0.17       |
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG13 | 20                  | 0.17     | 0.03                | 0.17       |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG11 | 20                  | 0.17     | 0.03                | 0.17       |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG12 | 20                  | 0.17     | 0.03                | 0.17       |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG13 | 20                  | 0.17     | 0.03                | 0.17       |
| (1,776)  | 1:52:A:ILE:HA   | 1:52:A:ILE:HD11 | 20                  | 0.17     | 0.01                | 0.17       |
| (1,776)  | 1:52:A:ILE:HA   | 1:52:A:ILE:HD12 | 20                  | 0.17     | 0.01                | 0.17       |
| (1,776)  | 1:52:A:ILE:HA   | 1:52:A:ILE:HD13 | 20                  | 0.17     | 0.01                | 0.17       |
| (1,49)   | 1:55:A:ARG:H    | 1:59:A:PRO:HA   | 20                  | 0.16     | 0.02                | 0.17       |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD21 | 20                  | 0.16     | 0.01                | 0.16       |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD22 | 20                  | 0.16     | 0.01                | 0.16       |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD23 | 20                  | 0.16     | 0.01                | 0.16       |
| (1,116)  | 1:44:A:ASP:H    | 1:44:A:ASP:HB3  | 20                  | 0.14     | 0.01                | 0.14       |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD11 | 19                  | 0.23     | 0.05                | 0.25       |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD12 | 19                  | 0.23     | 0.05                | 0.25       |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD13 | 19                  | 0.23     | 0.05                | 0.25       |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD1  | 19                  | 0.23     | 0.02                | 0.23       |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD2  | 19                  | 0.23     | 0.02                | 0.23       |
| (1,958)  | 1:29:A:GLU:HA   | 1:29:A:GLU:HG2  | 19                  | 0.18     | 0.03                | 0.17       |
| (1,958)  | 1:29:A:GLU:HA   | 1:29:A:GLU:HG3  | 19                  | 0.18     | 0.03                | 0.17       |
| (1,717)  | 1:53:A:VAL:HG11 | 1:60:A:TYR:HB3  | 19                  | 0.16     | 0.02                | 0.16       |
| (1,717)  | 1:53:A:VAL:HG12 | 1:60:A:TYR:HB3  | 19                  | 0.16     | 0.02                | 0.16       |
| (1,717)  | 1:53:A:VAL:HG13 | 1:60:A:TYR:HB3  | 19                  | 0.16     | 0.02                | 0.16       |
| (1,717)  | 1:53:A:VAL:HG21 | 1:60:A:TYR:HB3  | 19                  | 0.16     | 0.02                | 0.16       |
| (1,717)  | 1:53:A:VAL:HG22 | 1:60:A:TYR:HB3  | 19                  | 0.16     | 0.02                | 0.16       |
| (1,717)  | 1:53:A:VAL:HG23 | 1:60:A:TYR:HB3  | 19                  | 0.16     | 0.02                | 0.16       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,82)   | 1:54:A:TYR:H    | 1:59:A:PRO:HA   | 19                  | 0.15     | 0.02                | 0.15       |
| (1,306)  | 1:45:A:PHE:HZ   | 1:52:A:ILE:HD11 | 19                  | 0.13     | 0.02                | 0.13       |
| (1,306)  | 1:45:A:PHE:HZ   | 1:52:A:ILE:HD12 | 19                  | 0.13     | 0.02                | 0.13       |
| (1,306)  | 1:45:A:PHE:HZ   | 1:52:A:ILE:HD13 | 19                  | 0.13     | 0.02                | 0.13       |
| (1,1142) | 1:69:A:PHE:H    | 1:69:A:PHE:HB3  | 18                  | 0.17     | 0.03                | 0.17       |
| (1,401)  | 1:32:A:TYR:HD1  | 1:55:A:ARG:HG2  | 18                  | 0.14     | 0.03                | 0.14       |
| (1,401)  | 1:32:A:TYR:HD2  | 1:55:A:ARG:HG2  | 18                  | 0.14     | 0.03                | 0.14       |
| (1,850)  | 1:23:A:ILE:HA   | 1:23:A:ILE:HG13 | 18                  | 0.13     | 0.01                | 0.13       |
| (1,256)  | 1:9:A:PRO:HB3   | 1:11:A:LYS:H    | 17                  | 0.12     | 0.01                | 0.12       |
| (1,595)  | 1:16:A:CYS:HA   | 1:19:A:LEU:HB3  | 17                  | 0.12     | 0.02                | 0.11       |
| (1,628)  | 1:34:A:LYS:H    | 1:34:A:LYS:HG2  | 16                  | 0.19     | 0.04                | 0.2        |
| (1,625)  | 1:8:A:ARG:HG2   | 1:59:A:PRO:HG2  | 16                  | 0.15     | 0.03                | 0.15       |
| (1,625)  | 1:8:A:ARG:HG3   | 1:59:A:PRO:HG2  | 16                  | 0.15     | 0.03                | 0.15       |
| (1,1035) | 1:17:A:THR:HG21 | 1:18:A:GLU:HG3  | 16                  | 0.13     | 0.01                | 0.14       |
| (1,1035) | 1:17:A:THR:HG22 | 1:18:A:GLU:HG3  | 16                  | 0.13     | 0.01                | 0.14       |
| (1,1035) | 1:17:A:THR:HG23 | 1:18:A:GLU:HG3  | 16                  | 0.13     | 0.01                | 0.14       |
| (1,924)  | 1:9:A:PRO:HD2   | 1:15:A:LEU:HB3  | 15                  | 0.15     | 0.04                | 0.13       |
| (1,409)  | 1:78:A:HIS:HB2  | 1:78:A:HIS:HD2  | 15                  | 0.15     | 0.03                | 0.15       |
| (1,700)  | 1:19:A:LEU:H    | 1:19:A:LEU:HD21 | 15                  | 0.15     | 0.02                | 0.15       |
| (1,700)  | 1:19:A:LEU:H    | 1:19:A:LEU:HD22 | 15                  | 0.15     | 0.02                | 0.15       |
| (1,700)  | 1:19:A:LEU:H    | 1:19:A:LEU:HD23 | 15                  | 0.15     | 0.02                | 0.15       |
| (1,465)  | 1:32:A:TYR:HE1  | 1:55:A:ARG:HG2  | 15                  | 0.14     | 0.02                | 0.13       |
| (1,465)  | 1:32:A:TYR:HE2  | 1:55:A:ARG:HG2  | 15                  | 0.14     | 0.02                | 0.13       |
| (1,864)  | 1:69:A:PHE:HA   | 1:69:A:PHE:HB2  | 15                  | 0.13     | 0.01                | 0.13       |
| (1,1170) | 1:48:A:ARG:H    | 1:48:A:ARG:HD3  | 15                  | 0.12     | 0.02                | 0.12       |
| (1,984)  | 1:26:A:ILE:HG13 | 1:28:A:LEU:HA   | 15                  | 0.12     | 0.01                | 0.12       |
| (1,1118) | 1:7:A:GLU:HA    | 1:8:A:ARG:H     | 14                  | 0.16     | 0.05                | 0.15       |
| (1,1234) | 1:10:A:ARG:HA   | 1:52:A:ILE:HD11 | 14                  | 0.14     | 0.02                | 0.15       |
| (1,1234) | 1:10:A:ARG:HA   | 1:52:A:ILE:HD12 | 14                  | 0.14     | 0.02                | 0.15       |
| (1,1234) | 1:10:A:ARG:HA   | 1:52:A:ILE:HD13 | 14                  | 0.14     | 0.02                | 0.15       |
| (1,467)  | 1:54:A:TYR:HE1  | 1:58:A:ASN:HA   | 14                  | 0.13     | 0.02                | 0.13       |
| (1,467)  | 1:54:A:TYR:HE2  | 1:58:A:ASN:HA   | 14                  | 0.13     | 0.02                | 0.13       |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG11 | 14                  | 0.12     | 0.01                | 0.12       |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG12 | 14                  | 0.12     | 0.01                | 0.12       |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG13 | 14                  | 0.12     | 0.01                | 0.12       |
| (1,464)  | 1:32:A:TYR:HA   | 1:32:A:TYR:HE1  | 14                  | 0.12     | 0.02                | 0.12       |
| (1,464)  | 1:32:A:TYR:HA   | 1:32:A:TYR:HE2  | 14                  | 0.12     | 0.02                | 0.12       |
| (1,1064) | 1:26:A:ILE:HD11 | 1:28:A:LEU:HA   | 14                  | 0.11     | 0.01                | 0.11       |
| (1,1064) | 1:26:A:ILE:HD12 | 1:28:A:LEU:HA   | 14                  | 0.11     | 0.01                | 0.11       |
| (1,1064) | 1:26:A:ILE:HD13 | 1:28:A:LEU:HA   | 14                  | 0.11     | 0.01                | 0.11       |
| (1,430)  | 1:3:A:GLN:HA    | 1:3:A:GLN:HE22  | 13                  | 0.2      | 0.05                | 0.2        |
| (1,556)  | 1:29:A:GLU:HG2  | 1:60:A:TYR:HB2  | 13                  | 0.18     | 0.06                | 0.16       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,556)  | 1:29:A:GLU:HG3  | 1:60:A:TYR:HB2  | 13                  | 0.18     | 0.06                | 0.16       |
| (1,538)  | 1:18:A:GLU:HB3  | 1:19:A:LEU:H    | 13                  | 0.13     | 0.02                | 0.13       |
| (1,459)  | 1:50:A:LEU:H    | 1:50:A:LEU:HG   | 13                  | 0.13     | 0.01                | 0.13       |
| (1,1225) | 1:2:A:PHE:HE1   | 1:54:A:TYR:HE1  | 13                  | 0.12     | 0.02                | 0.12       |
| (1,1225) | 1:2:A:PHE:HE1   | 1:54:A:TYR:HE2  | 13                  | 0.12     | 0.02                | 0.12       |
| (1,1225) | 1:2:A:PHE:HE2   | 1:54:A:TYR:HE1  | 13                  | 0.12     | 0.02                | 0.12       |
| (1,1225) | 1:2:A:PHE:HE2   | 1:54:A:TYR:HE2  | 13                  | 0.12     | 0.02                | 0.12       |
| (1,1108) | 1:52:A:ILE:HD11 | 1:61:A:ALA:H    | 13                  | 0.12     | 0.01                | 0.12       |
| (1,1108) | 1:52:A:ILE:HD12 | 1:61:A:ALA:H    | 13                  | 0.12     | 0.01                | 0.12       |
| (1,1108) | 1:52:A:ILE:HD13 | 1:61:A:ALA:H    | 13                  | 0.12     | 0.01                | 0.12       |
| (1,576)  | 1:40:A:ARG:H    | 1:40:A:ARG:HB3  | 13                  | 0.11     | 0.01                | 0.11       |
| (1,165)  | 1:35:A:GLN:H    | 1:35:A:GLN:HB2  | 12                  | 0.22     | 0.04                | 0.2        |
| (1,1140) | 1:29:A:GLU:H    | 1:29:A:GLU:HB2  | 12                  | 0.12     | 0.01                | 0.12       |
| (1,741)  | 1:15:A:LEU:HG   | 1:16:A:CYS:HA   | 12                  | 0.11     | 0.01                | 0.11       |
| (1,358)  | 1:24:A:HIS:HB3  | 1:24:A:HIS:HD2  | 12                  | 0.11     | 0.01                | 0.11       |
| (1,97)   | 1:36:A:GLN:H    | 1:36:A:GLN:HB3  | 11                  | 0.21     | 0.03                | 0.2        |
| (1,1215) | 1:3:A:GLN:HE22  | 1:4:A:ASP:HA    | 11                  | 0.17     | 0.05                | 0.16       |
| (1,667)  | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD11 | 11                  | 0.13     | 0.01                | 0.13       |
| (1,667)  | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD12 | 11                  | 0.13     | 0.01                | 0.13       |
| (1,667)  | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD13 | 11                  | 0.13     | 0.01                | 0.13       |
| (1,667)  | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD11 | 11                  | 0.13     | 0.01                | 0.13       |
| (1,667)  | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD12 | 11                  | 0.13     | 0.01                | 0.13       |
| (1,667)  | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD13 | 11                  | 0.13     | 0.01                | 0.13       |
| (1,667)  | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD11 | 11                  | 0.13     | 0.01                | 0.13       |
| (1,667)  | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD12 | 11                  | 0.13     | 0.01                | 0.13       |
| (1,667)  | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD13 | 11                  | 0.13     | 0.01                | 0.13       |
| (1,575)  | 1:10:A:ARG:HA   | 1:10:A:ARG:HG3  | 10                  | 0.15     | 0.02                | 0.15       |
| (1,574)  | 1:11:A:LYS:HA   | 1:11:A:LYS:HD2  | 10                  | 0.13     | 0.02                | 0.13       |
| (1,574)  | 1:11:A:LYS:HA   | 1:11:A:LYS:HD3  | 10                  | 0.13     | 0.02                | 0.13       |
| (1,455)  | 1:54:A:TYR:HD1  | 1:59:A:PRO:HB2  | 10                  | 0.13     | 0.03                | 0.11       |
| (1,455)  | 1:54:A:TYR:HD2  | 1:59:A:PRO:HB2  | 10                  | 0.13     | 0.03                | 0.11       |
| (1,561)  | 1:39:A:ARG:HG2  | 1:43:A:TYR:HB2  | 10                  | 0.13     | 0.02                | 0.12       |
| (1,561)  | 1:39:A:ARG:HG2  | 1:43:A:TYR:HB3  | 10                  | 0.13     | 0.02                | 0.12       |
| (1,561)  | 1:39:A:ARG:HG3  | 1:43:A:TYR:HB2  | 10                  | 0.13     | 0.02                | 0.12       |
| (1,561)  | 1:39:A:ARG:HG3  | 1:43:A:TYR:HB3  | 10                  | 0.13     | 0.02                | 0.12       |
| (1,590)  | 1:13:A:PRO:HB3  | 1:46:A:ALA:HB1  | 10                  | 0.13     | 0.01                | 0.12       |
| (1,590)  | 1:13:A:PRO:HB3  | 1:46:A:ALA:HB2  | 10                  | 0.13     | 0.01                | 0.12       |
| (1,590)  | 1:13:A:PRO:HB3  | 1:46:A:ALA:HB3  | 10                  | 0.13     | 0.01                | 0.12       |
| (1,1203) | 1:35:A:GLN:HA   | 1:35:A:GLN:HE22 | 9                   | 0.25     | 0.07                | 0.27       |
| (1,126)  | 1:6:A:GLN:H     | 1:7:A:GLU:H     | 9                   | 0.24     | 0.06                | 0.25       |
| (1,1114) | 1:36:A:GLN:H    | 1:36:A:GLN:HG3  | 9                   | 0.15     | 0.03                | 0.14       |
| (1,599)  | 1:37:A:LEU:HA   | 1:38:A:LEU:HB3  | 9                   | 0.14     | 0.04                | 0.14       |

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| Key      | Atom-1          | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,1072) | 1:29:A:GLU:HB2  | 1:37:A:LEU:H   | 9                   | 0.13     | 0.03                | 0.12       |
| (1,867)  | 1:15:A:LEU:HD11 | 1:18:A:GLU:HA  | 9                   | 0.13     | 0.02                | 0.14       |
| (1,867)  | 1:15:A:LEU:HD12 | 1:18:A:GLU:HA  | 9                   | 0.13     | 0.02                | 0.14       |
| (1,867)  | 1:15:A:LEU:HD13 | 1:18:A:GLU:HA  | 9                   | 0.13     | 0.02                | 0.14       |
| (1,486)  | 1:43:A:TYR:HB2  | 1:47:A:ARG:HB3 | 9                   | 0.12     | 0.02                | 0.11       |
| (1,486)  | 1:43:A:TYR:HB3  | 1:47:A:ARG:HB3 | 9                   | 0.12     | 0.02                | 0.11       |
| (1,129)  | 1:5:A:PRO:HB3   | 1:6:A:GLN:H    | 8                   | 0.28     | 0.02                | 0.28       |
| (1,1057) | 1:1:A:MET:HE1   | 1:2:A:PHE:HA   | 8                   | 0.17     | 0.06                | 0.14       |
| (1,1057) | 1:1:A:MET:HE2   | 1:2:A:PHE:HA   | 8                   | 0.17     | 0.06                | 0.14       |
| (1,1057) | 1:1:A:MET:HE3   | 1:2:A:PHE:HA   | 8                   | 0.17     | 0.06                | 0.14       |
| (1,888)  | 1:44:A:ASP:HA   | 1:47:A:ARG:H   | 8                   | 0.14     | 0.02                | 0.14       |
| (1,964)  | 1:53:A:VAL:HG21 | 1:62:A:VAL:HB  | 8                   | 0.13     | 0.02                | 0.12       |
| (1,964)  | 1:53:A:VAL:HG22 | 1:62:A:VAL:HB  | 8                   | 0.13     | 0.02                | 0.12       |
| (1,964)  | 1:53:A:VAL:HG23 | 1:62:A:VAL:HB  | 8                   | 0.13     | 0.02                | 0.12       |
| (1,478)  | 1:8:A:ARG:HG2   | 1:59:A:PRO:HD2 | 8                   | 0.13     | 0.02                | 0.12       |
| (1,478)  | 1:8:A:ARG:HG3   | 1:59:A:PRO:HD2 | 8                   | 0.13     | 0.02                | 0.12       |
| (1,45)   | 1:36:A:GLN:HG3  | 1:37:A:LEU:H   | 8                   | 0.12     | 0.02                | 0.12       |
| (1,547)  | 1:8:A:ARG:HB2   | 1:59:A:PRO:HG3 | 7                   | 0.14     | 0.02                | 0.13       |
| (1,547)  | 1:8:A:ARG:HB3   | 1:59:A:PRO:HG3 | 7                   | 0.14     | 0.02                | 0.13       |
| (1,447)  | 1:43:A:TYR:H    | 1:43:A:TYR:HE1 | 7                   | 0.11     | 0.0                 | 0.11       |
| (1,447)  | 1:43:A:TYR:H    | 1:43:A:TYR:HE2 | 7                   | 0.11     | 0.0                 | 0.11       |
| (1,313)  | 1:2:A:PHE:H     | 1:2:A:PHE:HD1  | 6                   | 0.15     | 0.03                | 0.15       |
| (1,313)  | 1:2:A:PHE:H     | 1:2:A:PHE:HD2  | 6                   | 0.15     | 0.03                | 0.15       |
| (1,1228) | 1:9:A:PRO:HG2   | 1:54:A:TYR:HE1 | 6                   | 0.15     | 0.03                | 0.15       |
| (1,1228) | 1:9:A:PRO:HG2   | 1:54:A:TYR:HE2 | 6                   | 0.15     | 0.03                | 0.15       |
| (1,1228) | 1:9:A:PRO:HG3   | 1:54:A:TYR:HE1 | 6                   | 0.15     | 0.03                | 0.15       |
| (1,1228) | 1:9:A:PRO:HG3   | 1:54:A:TYR:HE2 | 6                   | 0.15     | 0.03                | 0.15       |
| (1,316)  | 1:2:A:PHE:HD1   | 1:9:A:PRO:HD3  | 6                   | 0.14     | 0.03                | 0.15       |
| (1,316)  | 1:2:A:PHE:HD2   | 1:9:A:PRO:HD3  | 6                   | 0.14     | 0.03                | 0.15       |
| (1,96)   | 1:35:A:GLN:HB2  | 1:36:A:GLN:H   | 6                   | 0.14     | 0.02                | 0.14       |
| (1,418)  | 1:29:A:GLU:HG2  | 1:60:A:TYR:HD1 | 6                   | 0.13     | 0.02                | 0.13       |
| (1,418)  | 1:29:A:GLU:HG2  | 1:60:A:TYR:HD2 | 6                   | 0.13     | 0.02                | 0.13       |
| (1,418)  | 1:29:A:GLU:HG3  | 1:60:A:TYR:HD1 | 6                   | 0.13     | 0.02                | 0.13       |
| (1,418)  | 1:29:A:GLU:HG3  | 1:60:A:TYR:HD2 | 6                   | 0.13     | 0.02                | 0.13       |
| (1,518)  | 1:40:A:ARG:H    | 1:41:A:GLU:HG2 | 6                   | 0.12     | 0.01                | 0.12       |
| (1,968)  | 1:35:A:GLN:H    | 1:35:A:GLN:HG2 | 5                   | 0.24     | 0.04                | 0.25       |
| (1,968)  | 1:35:A:GLN:H    | 1:35:A:GLN:HG3 | 5                   | 0.24     | 0.04                | 0.25       |
| (1,866)  | 1:65:A:LYS:HA   | 1:65:A:LYS:HG3 | 5                   | 0.2      | 0.02                | 0.2        |
| (1,996)  | 1:10:A:ARG:HA   | 1:10:A:ARG:HG2 | 5                   | 0.17     | 0.02                | 0.17       |
| (1,241)  | 1:34:A:LYS:H    | 1:34:A:LYS:HG3 | 5                   | 0.17     | 0.03                | 0.17       |
| (1,310)  | 1:2:A:PHE:HD1   | 1:8:A:ARG:H    | 5                   | 0.15     | 0.03                | 0.14       |
| (1,310)  | 1:2:A:PHE:HD2   | 1:8:A:ARG:H    | 5                   | 0.15     | 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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1177) | 1:19:A:LEU:H    | 1:19:A:LEU:HG   | 5                   | 0.13     | 0.02                | 0.13       |
| (1,578)  | 1:67:A:LEU:H    | 1:67:A:LEU:HG   | 5                   | 0.12     | 0.01                | 0.11       |
| (1,317)  | 1:24:A:HIS:HB3  | 1:25:A:ASP:H    | 5                   | 0.12     | 0.01                | 0.11       |
| (1,93)   | 1:29:A:GLU:HA   | 1:36:A:GLN:H    | 5                   | 0.11     | 0.01                | 0.11       |
| (1,1106) | 1:10:A:ARG:H    | 1:10:A:ARG:HB3  | 5                   | 0.11     | 0.01                | 0.11       |
| (1,664)  | 1:12:A:LEU:HD11 | 1:15:A:LEU:HB2  | 5                   | 0.11     | 0.01                | 0.1        |
| (1,664)  | 1:12:A:LEU:HD12 | 1:15:A:LEU:HB2  | 5                   | 0.11     | 0.01                | 0.1        |
| (1,664)  | 1:12:A:LEU:HD13 | 1:15:A:LEU:HB2  | 5                   | 0.11     | 0.01                | 0.1        |
| (1,1183) | 1:11:A:LYS:H    | 1:11:A:LYS:HB3  | 5                   | 0.11     | 0.01                | 0.1        |
| (1,223)  | 1:7:A:GLU:H     | 1:7:A:GLU:HB3   | 4                   | 0.19     | 0.05                | 0.18       |
| (1,26)   | 1:63:A:CYS:H    | 1:66:A:CYS:HB3  | 4                   | 0.15     | 0.06                | 0.13       |
| (1,321)  | 1:2:A:PHE:HD1   | 1:19:A:LEU:HG   | 4                   | 0.15     | 0.04                | 0.14       |
| (1,321)  | 1:2:A:PHE:HD2   | 1:19:A:LEU:HG   | 4                   | 0.15     | 0.04                | 0.14       |
| (1,932)  | 1:10:A:ARG:HA   | 1:10:A:ARG:HD2  | 4                   | 0.15     | 0.04                | 0.15       |
| (1,932)  | 1:10:A:ARG:HA   | 1:10:A:ARG:HD3  | 4                   | 0.15     | 0.04                | 0.15       |
| (1,381)  | 1:78:A:HIS:HB2  | 1:79:A:TYR:HD1  | 4                   | 0.14     | 0.01                | 0.14       |
| (1,381)  | 1:78:A:HIS:HB2  | 1:79:A:TYR:HD2  | 4                   | 0.14     | 0.01                | 0.14       |
| (1,505)  | 1:41:A:GLU:HA   | 1:44:A:ASP:HB3  | 4                   | 0.12     | 0.02                | 0.12       |
| (1,167)  | 1:74:A:SER:HA   | 1:75:A:GLU:H    | 4                   | 0.12     | 0.01                | 0.12       |
| (1,439)  | 1:79:A:TYR:HA   | 1:79:A:TYR:HE1  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,439)  | 1:79:A:TYR:HA   | 1:79:A:TYR:HE2  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,907)  | 1:77:A:ARG:HA   | 1:77:A:ARG:HG2  | 4                   | 0.11     | 0.01                | 0.11       |
| (1,907)  | 1:77:A:ARG:HA   | 1:77:A:ARG:HG3  | 4                   | 0.11     | 0.01                | 0.11       |
| (1,660)  | 1:12:A:LEU:HD11 | 1:61:A:ALA:HA   | 4                   | 0.11     | 0.01                | 0.11       |
| (1,660)  | 1:12:A:LEU:HD12 | 1:61:A:ALA:HA   | 4                   | 0.11     | 0.01                | 0.11       |
| (1,660)  | 1:12:A:LEU:HD13 | 1:61:A:ALA:HA   | 4                   | 0.11     | 0.01                | 0.11       |
| (1,541)  | 1:11:A:LYS:HB2  | 1:13:A:PRO:HD3  | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,510)  | 1:22:A:THR:HB   | 1:25:A:ASP:HB2  | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,461)  | 1:70:A:TYR:HA   | 1:70:A:TYR:HE1  | 4                   | 0.1      | 0.0                 | 0.1        |
| (1,461)  | 1:70:A:TYR:HA   | 1:70:A:TYR:HE2  | 4                   | 0.1      | 0.0                 | 0.1        |
| (1,1113) | 1:35:A:GLN:HG2  | 1:36:A:GLN:H    | 3                   | 0.23     | 0.0                 | 0.23       |
| (1,1113) | 1:35:A:GLN:HG3  | 1:36:A:GLN:H    | 3                   | 0.23     | 0.0                 | 0.23       |
| (1,724)  | 1:73:A:ILE:HA   | 1:73:A:ILE:HD11 | 3                   | 0.17     | 0.01                | 0.17       |
| (1,724)  | 1:73:A:ILE:HA   | 1:73:A:ILE:HD12 | 3                   | 0.17     | 0.01                | 0.17       |
| (1,724)  | 1:73:A:ILE:HA   | 1:73:A:ILE:HD13 | 3                   | 0.17     | 0.01                | 0.17       |
| (1,382)  | 1:78:A:HIS:HB3  | 1:79:A:TYR:HD1  | 3                   | 0.17     | 0.02                | 0.16       |
| (1,382)  | 1:78:A:HIS:HB3  | 1:79:A:TYR:HD2  | 3                   | 0.17     | 0.02                | 0.16       |
| (1,1099) | 1:77:A:ARG:H    | 1:78:A:HIS:HB3  | 3                   | 0.13     | 0.0                 | 0.13       |
| (1,348)  | 1:66:A:CYS:HA   | 1:69:A:PHE:HZ   | 3                   | 0.13     | 0.02                | 0.13       |
| (1,287)  | 1:7:A:GLU:HB2   | 1:8:A:ARG:H     | 3                   | 0.13     | 0.02                | 0.11       |
| (1,580)  | 1:40:A:ARG:H    | 1:40:A:ARG:HG2  | 3                   | 0.13     | 0.0                 | 0.13       |
| (1,580)  | 1:40:A:ARG:H    | 1:40:A:ARG:HG3  | 3                   | 0.13     | 0.0                 | 0.13       |

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| Key      | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1240) | 1:41:A:GLU:HG2 | 1:64:A:ASP:HB2  | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,493)  | 1:65:A:LYS:HB2 | 1:65:A:LYS:HE2  | 3                   | 0.12     | 0.01                | 0.11       |
| (1,493)  | 1:65:A:LYS:HB2 | 1:65:A:LYS:HE3  | 3                   | 0.12     | 0.01                | 0.11       |
| (1,706)  | 1:23:A:ILE:HA  | 1:23:A:ILE:HD11 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,706)  | 1:23:A:ILE:HA  | 1:23:A:ILE:HD12 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,706)  | 1:23:A:ILE:HA  | 1:23:A:ILE:HD13 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1152) | 1:70:A:TYR:H   | 1:70:A:TYR:HB3  | 3                   | 0.11     | 0.01                | 0.11       |
| (1,14)   | 1:38:A:LEU:H   | 1:41:A:GLU:HB3  | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,235)  | 1:30:A:CYS:HB2 | 1:34:A:LYS:H    | 3                   | 0.11     | 0.01                | 0.1        |
| (1,584)  | 1:22:A:THR:HB  | 1:23:A:ILE:HB   | 3                   | 0.11     | 0.01                | 0.1        |
| (1,480)  | 1:46:A:ALA:H   | 1:47:A:ARG:HD2  | 2                   | 0.22     | 0.08                | 0.22       |
| (1,480)  | 1:46:A:ALA:H   | 1:47:A:ARG:HD3  | 2                   | 0.22     | 0.08                | 0.22       |
| (1,961)  | 1:7:A:GLU:HA   | 1:7:A:GLU:HG2   | 2                   | 0.22     | 0.02                | 0.22       |
| (1,760)  | 1:48:A:ARG:HD3 | 1:50:A:LEU:HD21 | 2                   | 0.2      | 0.0                 | 0.2        |
| (1,760)  | 1:48:A:ARG:HD3 | 1:50:A:LEU:HD22 | 2                   | 0.2      | 0.0                 | 0.2        |
| (1,760)  | 1:48:A:ARG:HD3 | 1:50:A:LEU:HD23 | 2                   | 0.2      | 0.0                 | 0.2        |
| (1,966)  | 1:33:A:CYS:HB2 | 1:35:A:GLN:HG2  | 2                   | 0.18     | 0.0                 | 0.18       |
| (1,966)  | 1:33:A:CYS:HB2 | 1:35:A:GLN:HG3  | 2                   | 0.18     | 0.0                 | 0.18       |
| (1,905)  | 1:77:A:ARG:HA  | 1:77:A:ARG:HD2  | 2                   | 0.16     | 0.04                | 0.16       |
| (1,905)  | 1:77:A:ARG:HA  | 1:77:A:ARG:HD3  | 2                   | 0.16     | 0.04                | 0.16       |
| (1,691)  | 1:18:A:GLU:HG3 | 1:19:A:LEU:HD11 | 2                   | 0.16     | 0.04                | 0.16       |
| (1,691)  | 1:18:A:GLU:HG3 | 1:19:A:LEU:HD12 | 2                   | 0.16     | 0.04                | 0.16       |
| (1,691)  | 1:18:A:GLU:HG3 | 1:19:A:LEU:HD13 | 2                   | 0.16     | 0.04                | 0.16       |
| (1,916)  | 1:8:A:ARG:HA   | 1:8:A:ARG:HG2   | 2                   | 0.16     | 0.01                | 0.16       |
| (1,916)  | 1:8:A:ARG:HA   | 1:8:A:ARG:HG3   | 2                   | 0.16     | 0.01                | 0.16       |
| (1,956)  | 1:18:A:GLU:H   | 1:18:A:GLU:HG2  | 2                   | 0.15     | 0.01                | 0.15       |
| (1,1145) | 1:73:A:ILE:H   | 1:73:A:ILE:HB   | 2                   | 0.14     | 0.02                | 0.14       |
| (1,207)  | 1:76:A:TYR:H   | 1:76:A:TYR:HD1  | 2                   | 0.14     | 0.02                | 0.14       |
| (1,207)  | 1:76:A:TYR:H   | 1:76:A:TYR:HD2  | 2                   | 0.14     | 0.02                | 0.14       |
| (1,407)  | 1:38:A:LEU:HB2 | 1:41:A:GLU:H    | 2                   | 0.13     | 0.0                 | 0.13       |
| (1,477)  | 1:77:A:ARG:H   | 1:78:A:HIS:HA   | 2                   | 0.13     | 0.01                | 0.13       |
| (1,1163) | 1:4:A:ASP:HA   | 1:6:A:GLN:H     | 2                   | 0.13     | 0.01                | 0.13       |
| (1,160)  | 1:35:A:GLN:H   | 1:35:A:GLN:HB3  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,239)  | 1:11:A:LYS:HD2 | 1:14:A:GLN:HE21 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,239)  | 1:11:A:LYS:HD3 | 1:14:A:GLN:HE21 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,292)  | 1:2:A:PHE:HA   | 1:2:A:PHE:HE1   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,292)  | 1:2:A:PHE:HA   | 1:2:A:PHE:HE2   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,522)  | 1:1:A:MET:HA   | 1:1:A:MET:HG2   | 2                   | 0.12     | 0.01                | 0.12       |
| (1,872)  | 1:73:A:ILE:HB  | 1:74:A:SER:HA   | 2                   | 0.12     | 0.01                | 0.12       |
| (1,753)  | 1:50:A:LEU:H   | 1:50:A:LEU:HD21 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,753)  | 1:50:A:LEU:H   | 1:50:A:LEU:HD22 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,753)  | 1:50:A:LEU:H   | 1:50:A:LEU:HD23 | 2                   | 0.12     | 0.01                | 0.12       |

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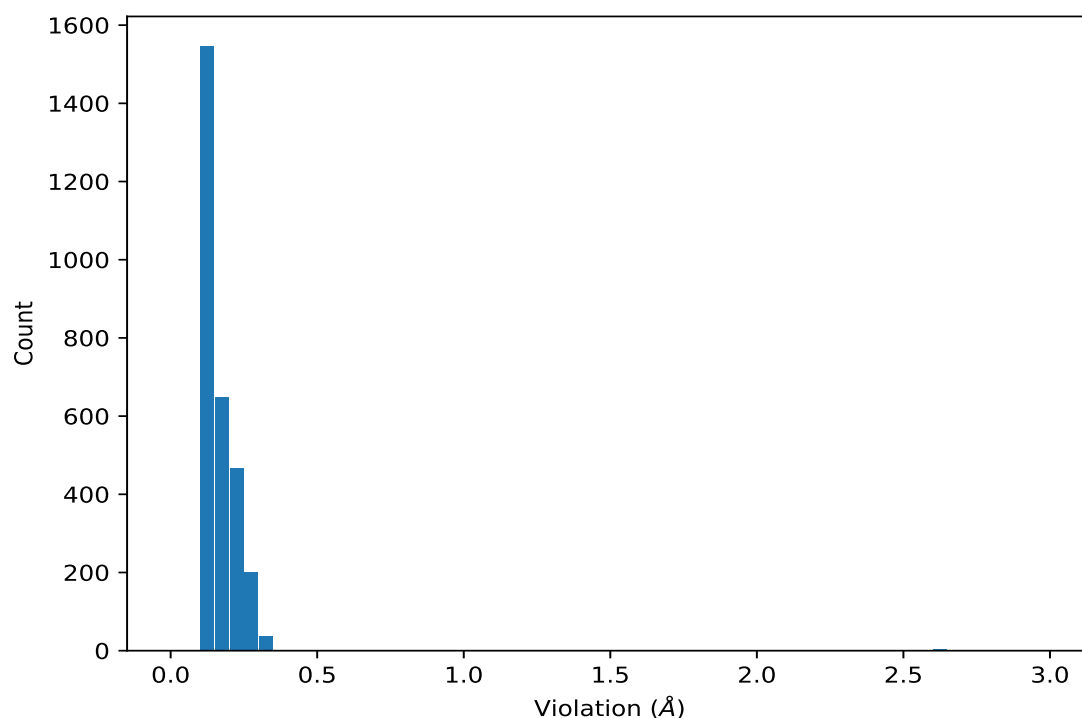
| Key      | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1218) | 1:3:A:GLN:HE21 | 1:4:A:ASP:HA    | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1227) | 1:2:A:PHE:HB3  | 1:54:A:TYR:HE1  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1227) | 1:2:A:PHE:HB3  | 1:54:A:TYR:HE2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,216)  | 1:46:A:ALA:HB1 | 1:48:A:ARG:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,216)  | 1:46:A:ALA:HB2 | 1:48:A:ARG:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,216)  | 1:46:A:ALA:HB3 | 1:48:A:ARG:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,606)  | 1:34:A:LYS:HA  | 1:34:A:LYS:HD3  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,745)  | 1:50:A:LEU:HA  | 1:50:A:LEU:HD11 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,745)  | 1:50:A:LEU:HA  | 1:50:A:LEU:HD12 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,745)  | 1:50:A:LEU:HA  | 1:50:A:LEU:HD13 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,47)   | 1:54:A:TYR:HD1 | 1:55:A:ARG:H    | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,47)   | 1:54:A:TYR:HD2 | 1:55:A:ARG:H    | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,962)  | 1:7:A:GLU:HA   | 1:7:A:GLU:HG3   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,734)  | 1:27:A:ILE:H   | 1:27:A:ILE:HG21 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,734)  | 1:27:A:ILE:H   | 1:27:A:ILE:HG22 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,734)  | 1:27:A:ILE:H   | 1:27:A:ILE:HG23 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1232) | 1:24:A:HIS:HA  | 1:43:A:TYR:HE1  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1232) | 1:24:A:HIS:HA  | 1:43:A:TYR:HE2  | 2                   | 0.11     | 0.0                 | 0.11       |

<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) |
|----------|----------------|-------------|----------|---------------|
| (1,1237) | 1:59:A:PRO:HD3 | 1:8:A:ARG:H | 7        | 3.0           |
| (1,1237) | 1:59:A:PRO:HD3 | 1:8:A:ARG:H | 5        | 2.91          |
| (1,1237) | 1:59:A:PRO:HD3 | 1:8:A:ARG:H | 16       | 2.9           |
| (1,1237) | 1:59:A:PRO:HD3 | 1:8:A:ARG:H | 12       | 2.87          |
| (1,1237) | 1:59:A:PRO:HD3 | 1:8:A:ARG:H | 13       | 2.83          |
| (1,1237) | 1:59:A:PRO:HD3 | 1:8:A:ARG:H | 10       | 2.8           |
| (1,1237) | 1:59:A:PRO:HD3 | 1:8:A:ARG:H | 1        | 2.79          |
| (1,1237) | 1:59:A:PRO:HD3 | 1:8:A:ARG:H | 4        | 2.74          |
| (1,1237) | 1:59:A:PRO:HD3 | 1:8:A:ARG:H | 6        | 2.64          |
| (1,1237) | 1:59:A:PRO:HD3 | 1:8:A:ARG:H | 19       | 2.63          |
| (1,1237) | 1:59:A:PRO:HD3 | 1:8:A:ARG:H | 9        | 2.61          |
| (1,1237) | 1:59:A:PRO:HD3 | 1:8:A:ARG:H | 3        | 2.52          |
| (1,1237) | 1:59:A:PRO:HD3 | 1:8:A:ARG:H | 8        | 2.49          |
| (1,1237) | 1:59:A:PRO:HD3 | 1:8:A:ARG:H | 14       | 2.48          |
| (1,1237) | 1:59:A:PRO:HD3 | 1:8:A:ARG:H | 2        | 2.37          |
| (1,1237) | 1:59:A:PRO:HD3 | 1:8:A:ARG:H | 17       | 2.29          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1237) | 1:59:A:PRO:HD3 | 1:8:A:ARG:H     | 15       | 2.23          |
| (1,1237) | 1:59:A:PRO:HD3 | 1:8:A:ARG:H     | 20       | 1.97          |
| (1,1237) | 1:59:A:PRO:HD3 | 1:8:A:ARG:H     | 18       | 1.53          |
| (1,1237) | 1:59:A:PRO:HD3 | 1:8:A:ARG:H     | 11       | 1.52          |
| (1,126)  | 1:6:A:GLN:H    | 1:7:A:GLU:H     | 8        | 0.38          |
| (1,556)  | 1:29:A:GLU:HG2 | 1:60:A:TYR:HB2  | 16       | 0.33          |
| (1,556)  | 1:29:A:GLU:HG3 | 1:60:A:TYR:HB2  | 16       | 0.33          |
| (1,340)  | 1:44:A:ASP:HB2 | 1:45:A:PHE:HD1  | 13       | 0.33          |
| (1,340)  | 1:44:A:ASP:HB2 | 1:45:A:PHE:HD2  | 13       | 0.33          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD11 | 1        | 0.32          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD12 | 1        | 0.32          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD13 | 1        | 0.32          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD11 | 2        | 0.32          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD12 | 2        | 0.32          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD13 | 2        | 0.32          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD11 | 7        | 0.32          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD12 | 7        | 0.32          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD13 | 7        | 0.32          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD11 | 11       | 0.32          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD12 | 11       | 0.32          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD13 | 11       | 0.32          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD11 | 13       | 0.32          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD12 | 13       | 0.32          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD13 | 13       | 0.32          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD11 | 16       | 0.32          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD12 | 16       | 0.32          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD13 | 16       | 0.32          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD11 | 20       | 0.32          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD12 | 20       | 0.32          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD13 | 20       | 0.32          |
| (1,1203) | 1:35:A:GLN:HA  | 1:35:A:GLN:HE22 | 10       | 0.31          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD11 | 6        | 0.31          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD12 | 6        | 0.31          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD13 | 6        | 0.31          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD11 | 14       | 0.31          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD12 | 14       | 0.31          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD13 | 14       | 0.31          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD11 | 15       | 0.31          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD12 | 15       | 0.31          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD13 | 15       | 0.31          |
| (1,340)  | 1:44:A:ASP:HB2 | 1:45:A:PHE:HD1  | 11       | 0.31          |
| (1,340)  | 1:44:A:ASP:HB2 | 1:45:A:PHE:HD2  | 11       | 0.31          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,129)  | 1:5:A:PRO:HB3  | 1:6:A:GLN:H     | 16       | 0.31          |
| (1,1203) | 1:35:A:GLN:HA  | 1:35:A:GLN:HE22 | 5        | 0.3           |
| (1,1203) | 1:35:A:GLN:HA  | 1:35:A:GLN:HE22 | 13       | 0.3           |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD11 | 4        | 0.3           |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD12 | 4        | 0.3           |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD13 | 4        | 0.3           |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD11 | 5        | 0.3           |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD12 | 5        | 0.3           |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD13 | 5        | 0.3           |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD11 | 10       | 0.3           |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD12 | 10       | 0.3           |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD13 | 10       | 0.3           |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD11 | 17       | 0.3           |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD12 | 17       | 0.3           |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD13 | 17       | 0.3           |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD11 | 18       | 0.3           |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD12 | 18       | 0.3           |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD13 | 18       | 0.3           |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD11 | 19       | 0.3           |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD12 | 19       | 0.3           |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD13 | 19       | 0.3           |
| (1,968)  | 1:35:A:GLN:H   | 1:35:A:GLN:HG2  | 17       | 0.3           |
| (1,968)  | 1:35:A:GLN:H   | 1:35:A:GLN:HG3  | 17       | 0.3           |
| (1,480)  | 1:46:A:ALA:H   | 1:47:A:ARG:HD2  | 10       | 0.3           |
| (1,480)  | 1:46:A:ALA:H   | 1:47:A:ARG:HD3  | 10       | 0.3           |
| (1,224)  | 1:7:A:GLU:H    | 1:8:A:ARG:H     | 18       | 0.3           |
| (1,1244) | 1:30:A:CYS:H   | 1:63:A:CYS:H    | 7        | 0.29          |
| (1,1203) | 1:35:A:GLN:HA  | 1:35:A:GLN:HE22 | 1        | 0.29          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD11 | 3        | 0.29          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD12 | 3        | 0.29          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD13 | 3        | 0.29          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD11 | 9        | 0.29          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD12 | 9        | 0.29          |
| (1,1030) | 1:27:A:ILE:HA  | 1:28:A:LEU:HD13 | 9        | 0.29          |
| (1,958)  | 1:29:A:GLU:HA  | 1:29:A:GLU:HG2  | 6        | 0.29          |
| (1,958)  | 1:29:A:GLU:HA  | 1:29:A:GLU:HG3  | 6        | 0.29          |
| (1,556)  | 1:29:A:GLU:HG2 | 1:60:A:TYR:HB2  | 4        | 0.29          |
| (1,556)  | 1:29:A:GLU:HG3 | 1:60:A:TYR:HB2  | 4        | 0.29          |
| (1,129)  | 1:5:A:PRO:HB3  | 1:6:A:GLN:H     | 1        | 0.29          |
| (1,129)  | 1:5:A:PRO:HB3  | 1:6:A:GLN:H     | 3        | 0.29          |
| (1,129)  | 1:5:A:PRO:HB3  | 1:6:A:GLN:H     | 9        | 0.29          |
| (1,1229) | 1:55:A:ARG:HG3 | 1:32:A:TYR:H    | 12       | 0.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1056) | 1:31:A:VAL:HG11 | 1:55:A:ARG:HA   | 3        | 0.28          |
| (1,1056) | 1:31:A:VAL:HG12 | 1:55:A:ARG:HA   | 3        | 0.28          |
| (1,1056) | 1:31:A:VAL:HG13 | 1:55:A:ARG:HA   | 3        | 0.28          |
| (1,1056) | 1:31:A:VAL:HG11 | 1:55:A:ARG:HA   | 4        | 0.28          |
| (1,1056) | 1:31:A:VAL:HG12 | 1:55:A:ARG:HA   | 4        | 0.28          |
| (1,1056) | 1:31:A:VAL:HG13 | 1:55:A:ARG:HA   | 4        | 0.28          |
| (1,1030) | 1:27:A:ILE:HA   | 1:28:A:LEU:HD11 | 8        | 0.28          |
| (1,1030) | 1:27:A:ILE:HA   | 1:28:A:LEU:HD12 | 8        | 0.28          |
| (1,1030) | 1:27:A:ILE:HA   | 1:28:A:LEU:HD13 | 8        | 0.28          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD11 | 8        | 0.28          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD12 | 8        | 0.28          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD13 | 8        | 0.28          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD11 | 15       | 0.28          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD12 | 15       | 0.28          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD13 | 15       | 0.28          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD11 | 16       | 0.28          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD12 | 16       | 0.28          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD13 | 16       | 0.28          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD11 | 19       | 0.28          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD12 | 19       | 0.28          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD13 | 19       | 0.28          |
| (1,430)  | 1:3:A:GLN:HA    | 1:3:A:GLN:HE22  | 10       | 0.28          |
| (1,165)  | 1:35:A:GLN:H    | 1:35:A:GLN:HB2  | 8        | 0.28          |
| (1,1244) | 1:30:A:CYS:H    | 1:63:A:CYS:H    | 12       | 0.27          |
| (1,1242) | 1:29:A:GLU:HB2  | 1:60:A:TYR:HB2  | 5        | 0.27          |
| (1,1203) | 1:35:A:GLN:HA   | 1:35:A:GLN:HE22 | 7        | 0.27          |
| (1,1203) | 1:35:A:GLN:HA   | 1:35:A:GLN:HE22 | 12       | 0.27          |
| (1,1057) | 1:1:A:MET:HE1   | 1:2:A:PHE:HA    | 16       | 0.27          |
| (1,1057) | 1:1:A:MET:HE2   | 1:2:A:PHE:HA    | 16       | 0.27          |
| (1,1057) | 1:1:A:MET:HE3   | 1:2:A:PHE:HA    | 16       | 0.27          |
| (1,1056) | 1:31:A:VAL:HG11 | 1:55:A:ARG:HA   | 6        | 0.27          |
| (1,1056) | 1:31:A:VAL:HG12 | 1:55:A:ARG:HA   | 6        | 0.27          |
| (1,1056) | 1:31:A:VAL:HG13 | 1:55:A:ARG:HA   | 6        | 0.27          |
| (1,1030) | 1:27:A:ILE:HA   | 1:28:A:LEU:HD11 | 12       | 0.27          |
| (1,1030) | 1:27:A:ILE:HA   | 1:28:A:LEU:HD12 | 12       | 0.27          |
| (1,1030) | 1:27:A:ILE:HA   | 1:28:A:LEU:HD13 | 12       | 0.27          |
| (1,968)  | 1:35:A:GLN:H    | 1:35:A:GLN:HG2  | 14       | 0.27          |
| (1,968)  | 1:35:A:GLN:H    | 1:35:A:GLN:HG3  | 14       | 0.27          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD11 | 10       | 0.27          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD12 | 10       | 0.27          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD13 | 10       | 0.27          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD11 | 20       | 0.27          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD12 | 20       | 0.27          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD13 | 20       | 0.27          |
| (1,649)  | 1:52:A:ILE:HA   | 1:62:A:VAL:HG21 | 16       | 0.27          |
| (1,649)  | 1:52:A:ILE:HA   | 1:62:A:VAL:HG22 | 16       | 0.27          |
| (1,649)  | 1:52:A:ILE:HA   | 1:62:A:VAL:HG23 | 16       | 0.27          |
| (1,340)  | 1:44:A:ASP:HB2  | 1:45:A:PHE:HD1  | 12       | 0.27          |
| (1,340)  | 1:44:A:ASP:HB2  | 1:45:A:PHE:HD2  | 12       | 0.27          |
| (1,223)  | 1:7:A:GLU:H     | 1:7:A:GLU:HB3   | 8        | 0.27          |
| (1,165)  | 1:35:A:GLN:H    | 1:35:A:GLN:HB2  | 19       | 0.27          |
| (1,129)  | 1:5:A:PRO:HB3   | 1:6:A:GLN:H     | 4        | 0.27          |
| (1,129)  | 1:5:A:PRO:HB3   | 1:6:A:GLN:H     | 8        | 0.27          |
| (1,126)  | 1:6:A:GLN:H     | 1:7:A:GLU:H     | 4        | 0.27          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB1  | 16       | 0.26          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB2  | 16       | 0.26          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB3  | 16       | 0.26          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB1  | 16       | 0.26          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB2  | 16       | 0.26          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB3  | 16       | 0.26          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB1  | 16       | 0.26          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB2  | 16       | 0.26          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB3  | 16       | 0.26          |
| (1,1242) | 1:29:A:GLU:HB2  | 1:60:A:TYR:HB2  | 8        | 0.26          |
| (1,1215) | 1:3:A:GLN:HE22  | 1:4:A:ASP:HA    | 16       | 0.26          |
| (1,1056) | 1:31:A:VAL:HG11 | 1:55:A:ARG:HA   | 10       | 0.26          |
| (1,1056) | 1:31:A:VAL:HG12 | 1:55:A:ARG:HA   | 10       | 0.26          |
| (1,1056) | 1:31:A:VAL:HG13 | 1:55:A:ARG:HA   | 10       | 0.26          |
| (1,1056) | 1:31:A:VAL:HG11 | 1:55:A:ARG:HA   | 16       | 0.26          |
| (1,1056) | 1:31:A:VAL:HG12 | 1:55:A:ARG:HA   | 16       | 0.26          |
| (1,1056) | 1:31:A:VAL:HG13 | 1:55:A:ARG:HA   | 16       | 0.26          |
| (1,1056) | 1:31:A:VAL:HG11 | 1:55:A:ARG:HA   | 18       | 0.26          |
| (1,1056) | 1:31:A:VAL:HG12 | 1:55:A:ARG:HA   | 18       | 0.26          |
| (1,1056) | 1:31:A:VAL:HG13 | 1:55:A:ARG:HA   | 18       | 0.26          |
| (1,1056) | 1:31:A:VAL:HG11 | 1:55:A:ARG:HA   | 19       | 0.26          |
| (1,1056) | 1:31:A:VAL:HG12 | 1:55:A:ARG:HA   | 19       | 0.26          |
| (1,1056) | 1:31:A:VAL:HG13 | 1:55:A:ARG:HA   | 19       | 0.26          |
| (1,1056) | 1:31:A:VAL:HG11 | 1:55:A:ARG:HA   | 20       | 0.26          |
| (1,1056) | 1:31:A:VAL:HG12 | 1:55:A:ARG:HA   | 20       | 0.26          |
| (1,1056) | 1:31:A:VAL:HG13 | 1:55:A:ARG:HA   | 20       | 0.26          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD11 | 2        | 0.26          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD12 | 2        | 0.26          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD13 | 2        | 0.26          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD11 | 11       | 0.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD12 | 11       | 0.26          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD13 | 11       | 0.26          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD11 | 14       | 0.26          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD12 | 14       | 0.26          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD13 | 14       | 0.26          |
| (1,430)  | 1:3:A:GLN:HA    | 1:3:A:GLN:HE22  | 6        | 0.26          |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD1  | 5        | 0.26          |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD2  | 5        | 0.26          |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD1  | 18       | 0.26          |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD2  | 18       | 0.26          |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD1  | 20       | 0.26          |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD2  | 20       | 0.26          |
| (1,340)  | 1:44:A:ASP:HB2  | 1:45:A:PHE:HD1  | 6        | 0.26          |
| (1,340)  | 1:44:A:ASP:HB2  | 1:45:A:PHE:HD2  | 6        | 0.26          |
| (1,165)  | 1:35:A:GLN:H    | 1:35:A:GLN:HB2  | 6        | 0.26          |
| (1,126)  | 1:6:A:GLN:H     | 1:7:A:GLU:H     | 1        | 0.26          |
| (1,126)  | 1:6:A:GLN:H     | 1:7:A:GLU:H     | 3        | 0.26          |
| (1,97)   | 1:36:A:GLN:H    | 1:36:A:GLN:HB3  | 11       | 0.26          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB1  | 3        | 0.25          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB2  | 3        | 0.25          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB3  | 3        | 0.25          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB1  | 3        | 0.25          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB2  | 3        | 0.25          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB3  | 3        | 0.25          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB1  | 3        | 0.25          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB2  | 3        | 0.25          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB3  | 3        | 0.25          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB1  | 12       | 0.25          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB2  | 12       | 0.25          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB3  | 12       | 0.25          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB1  | 12       | 0.25          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB2  | 12       | 0.25          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB3  | 12       | 0.25          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB1  | 12       | 0.25          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB2  | 12       | 0.25          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB3  | 12       | 0.25          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB1  | 18       | 0.25          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB2  | 18       | 0.25          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB3  | 18       | 0.25          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB1  | 18       | 0.25          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB2  | 18       | 0.25          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB3  | 18       | 0.25          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB1  | 18       | 0.25          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB2  | 18       | 0.25          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB3  | 18       | 0.25          |
| (1,1244) | 1:30:A:CYS:H    | 1:63:A:CYS:H    | 8        | 0.25          |
| (1,1244) | 1:30:A:CYS:H    | 1:63:A:CYS:H    | 16       | 0.25          |
| (1,1242) | 1:29:A:GLU:HB2  | 1:60:A:TYR:HB2  | 12       | 0.25          |
| (1,1229) | 1:55:A:ARG:HG3  | 1:32:A:TYR:H    | 1        | 0.25          |
| (1,1203) | 1:35:A:GLN:HA   | 1:35:A:GLN:HE22 | 4        | 0.25          |
| (1,1056) | 1:31:A:VAL:HG11 | 1:55:A:ARG:HA   | 8        | 0.25          |
| (1,1056) | 1:31:A:VAL:HG12 | 1:55:A:ARG:HA   | 8        | 0.25          |
| (1,1056) | 1:31:A:VAL:HG13 | 1:55:A:ARG:HA   | 8        | 0.25          |
| (1,1056) | 1:31:A:VAL:HG11 | 1:55:A:ARG:HA   | 11       | 0.25          |
| (1,1056) | 1:31:A:VAL:HG12 | 1:55:A:ARG:HA   | 11       | 0.25          |
| (1,1056) | 1:31:A:VAL:HG13 | 1:55:A:ARG:HA   | 11       | 0.25          |
| (1,968)  | 1:35:A:GLN:H    | 1:35:A:GLN:HG2  | 3        | 0.25          |
| (1,968)  | 1:35:A:GLN:H    | 1:35:A:GLN:HG3  | 3        | 0.25          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD11 | 4        | 0.25          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD12 | 4        | 0.25          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD13 | 4        | 0.25          |
| (1,628)  | 1:34:A:LYS:H    | 1:34:A:LYS:HG2  | 7        | 0.25          |
| (1,628)  | 1:34:A:LYS:H    | 1:34:A:LYS:HG2  | 16       | 0.25          |
| (1,430)  | 1:3:A:GLN:HA    | 1:3:A:GLN:HE22  | 17       | 0.25          |
| (1,423)  | 1:28:A:LEU:HA   | 1:60:A:TYR:HD1  | 16       | 0.25          |
| (1,423)  | 1:28:A:LEU:HA   | 1:60:A:TYR:HD2  | 16       | 0.25          |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD1  | 7        | 0.25          |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD2  | 7        | 0.25          |
| (1,340)  | 1:44:A:ASP:HB2  | 1:45:A:PHE:HD1  | 14       | 0.25          |
| (1,340)  | 1:44:A:ASP:HB2  | 1:45:A:PHE:HD2  | 14       | 0.25          |
| (1,165)  | 1:35:A:GLN:H    | 1:35:A:GLN:HB2  | 2        | 0.25          |
| (1,129)  | 1:5:A:PRO:HB3   | 1:6:A:GLN:H     | 19       | 0.25          |
| (1,126)  | 1:6:A:GLN:H     | 1:7:A:GLU:H     | 5        | 0.25          |
| (1,97)   | 1:36:A:GLN:H    | 1:36:A:GLN:HB3  | 16       | 0.25          |
| (1,26)   | 1:63:A:CYS:H    | 1:66:A:CYS:HB3  | 8        | 0.25          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB1  | 1        | 0.24          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB2  | 1        | 0.24          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB3  | 1        | 0.24          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB1  | 1        | 0.24          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB2  | 1        | 0.24          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB3  | 1        | 0.24          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB1  | 1        | 0.24          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB2  | 1        | 0.24          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB3  | 1        | 0.24          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB1 | 6        | 0.24          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB2 | 6        | 0.24          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB3 | 6        | 0.24          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB1 | 6        | 0.24          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB2 | 6        | 0.24          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB3 | 6        | 0.24          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB1 | 6        | 0.24          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB2 | 6        | 0.24          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB3 | 6        | 0.24          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB1 | 13       | 0.24          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB2 | 13       | 0.24          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB3 | 13       | 0.24          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB1 | 13       | 0.24          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB2 | 13       | 0.24          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB3 | 13       | 0.24          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB1 | 13       | 0.24          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB2 | 13       | 0.24          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB3 | 13       | 0.24          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB1 | 14       | 0.24          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB2 | 14       | 0.24          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB3 | 14       | 0.24          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB1 | 14       | 0.24          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB2 | 14       | 0.24          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB3 | 14       | 0.24          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB1 | 14       | 0.24          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB2 | 14       | 0.24          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB3 | 14       | 0.24          |
| (1,1244) | 1:30:A:CYS:H    | 1:63:A:CYS:H   | 13       | 0.24          |
| (1,1244) | 1:30:A:CYS:H    | 1:63:A:CYS:H   | 14       | 0.24          |
| (1,1118) | 1:7:A:GLU:HA    | 1:8:A:ARG:H    | 4        | 0.24          |
| (1,1118) | 1:7:A:GLU:HA    | 1:8:A:ARG:H    | 8        | 0.24          |
| (1,1113) | 1:35:A:GLN:HG2  | 1:36:A:GLN:H   | 11       | 0.24          |
| (1,1113) | 1:35:A:GLN:HG3  | 1:36:A:GLN:H   | 11       | 0.24          |
| (1,1057) | 1:1:A:MET:HE1   | 1:2:A:PHE:HA   | 13       | 0.24          |
| (1,1057) | 1:1:A:MET:HE2   | 1:2:A:PHE:HA   | 13       | 0.24          |
| (1,1057) | 1:1:A:MET:HE3   | 1:2:A:PHE:HA   | 13       | 0.24          |
| (1,1056) | 1:31:A:VAL:HG11 | 1:55:A:ARG:HA  | 2        | 0.24          |
| (1,1056) | 1:31:A:VAL:HG12 | 1:55:A:ARG:HA  | 2        | 0.24          |
| (1,1056) | 1:31:A:VAL:HG13 | 1:55:A:ARG:HA  | 2        | 0.24          |
| (1,1056) | 1:31:A:VAL:HG11 | 1:55:A:ARG:HA  | 12       | 0.24          |
| (1,1056) | 1:31:A:VAL:HG12 | 1:55:A:ARG:HA  | 12       | 0.24          |
| (1,1056) | 1:31:A:VAL:HG13 | 1:55:A:ARG:HA  | 12       | 0.24          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD11 | 5        | 0.24          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD12 | 5        | 0.24          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD13 | 5        | 0.24          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD11 | 12       | 0.24          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD12 | 12       | 0.24          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD13 | 12       | 0.24          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD11 | 13       | 0.24          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD12 | 13       | 0.24          |
| (1,689)  | 1:67:A:LEU:HA   | 1:67:A:LEU:HD13 | 13       | 0.24          |
| (1,649)  | 1:52:A:ILE:HA   | 1:62:A:VAL:HG21 | 8        | 0.24          |
| (1,649)  | 1:52:A:ILE:HA   | 1:62:A:VAL:HG22 | 8        | 0.24          |
| (1,649)  | 1:52:A:ILE:HA   | 1:62:A:VAL:HG23 | 8        | 0.24          |
| (1,628)  | 1:34:A:LYS:H    | 1:34:A:LYS:HG2  | 6        | 0.24          |
| (1,628)  | 1:34:A:LYS:H    | 1:34:A:LYS:HG2  | 10       | 0.24          |
| (1,599)  | 1:37:A:LEU:HA   | 1:38:A:LEU:HB3  | 11       | 0.24          |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD1  | 19       | 0.24          |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD2  | 19       | 0.24          |
| (1,340)  | 1:44:A:ASP:HB2  | 1:45:A:PHE:HD1  | 2        | 0.24          |
| (1,340)  | 1:44:A:ASP:HB2  | 1:45:A:PHE:HD2  | 2        | 0.24          |
| (1,340)  | 1:44:A:ASP:HB2  | 1:45:A:PHE:HD1  | 8        | 0.24          |
| (1,340)  | 1:44:A:ASP:HB2  | 1:45:A:PHE:HD2  | 8        | 0.24          |
| (1,129)  | 1:5:A:PRO:HB3   | 1:6:A:GLN:H     | 18       | 0.24          |
| (1,97)   | 1:36:A:GLN:H    | 1:36:A:GLN:HB3  | 9        | 0.24          |
| (1,53)   | 1:37:A:LEU:H    | 1:37:A:LEU:HB3  | 7        | 0.24          |
| (1,1253) | 1:32:A:TYR:HE1  | 1:62:A:VAL:HB   | 13       | 0.23          |
| (1,1253) | 1:32:A:TYR:HE2  | 1:62:A:VAL:HB   | 13       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB1  | 4        | 0.23          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB2  | 4        | 0.23          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB3  | 4        | 0.23          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB1  | 4        | 0.23          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB2  | 4        | 0.23          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB3  | 4        | 0.23          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB1  | 4        | 0.23          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB2  | 4        | 0.23          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB3  | 4        | 0.23          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB1  | 7        | 0.23          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB2  | 7        | 0.23          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB3  | 7        | 0.23          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB1  | 7        | 0.23          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB2  | 7        | 0.23          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB3  | 7        | 0.23          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB1  | 7        | 0.23          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB2 | 7        | 0.23          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB3 | 7        | 0.23          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB1 | 10       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB2 | 10       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB3 | 10       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB1 | 10       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB2 | 10       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB3 | 10       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB1 | 10       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB2 | 10       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB3 | 10       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB1 | 15       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB2 | 15       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB3 | 15       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB1 | 15       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB2 | 15       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB3 | 15       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB1 | 15       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB2 | 15       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB3 | 15       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB1 | 19       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB2 | 19       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB3 | 19       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB1 | 19       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB2 | 19       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB3 | 19       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB1 | 19       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB2 | 19       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB3 | 19       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB1 | 20       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB2 | 20       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB3 | 20       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB1 | 20       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB2 | 20       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB3 | 20       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB1 | 20       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB2 | 20       | 0.23          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB3 | 20       | 0.23          |
| (1,1244) | 1:30:A:CYS:H    | 1:63:A:CYS:H   | 4        | 0.23          |
| (1,1244) | 1:30:A:CYS:H    | 1:63:A:CYS:H   | 5        | 0.23          |
| (1,1244) | 1:30:A:CYS:H    | 1:63:A:CYS:H   | 19       | 0.23          |
| (1,1242) | 1:29:A:GLU:HB2  | 1:60:A:TYR:HB2 | 2        | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1242) | 1:29:A:GLU:HB2  | 1:60:A:TYR:HB2  | 15       | 0.23          |
| (1,1229) | 1:55:A:ARG:HG3  | 1:32:A:TYR:H    | 5        | 0.23          |
| (1,1229) | 1:55:A:ARG:HG3  | 1:32:A:TYR:H    | 7        | 0.23          |
| (1,1229) | 1:55:A:ARG:HG3  | 1:32:A:TYR:H    | 13       | 0.23          |
| (1,1229) | 1:55:A:ARG:HG3  | 1:32:A:TYR:H    | 16       | 0.23          |
| (1,1118) | 1:7:A:GLU:HA    | 1:8:A:ARG:H     | 7        | 0.23          |
| (1,1113) | 1:35:A:GLN:HG2  | 1:36:A:GLN:H    | 9        | 0.23          |
| (1,1113) | 1:35:A:GLN:HG3  | 1:36:A:GLN:H    | 9        | 0.23          |
| (1,1113) | 1:35:A:GLN:HG2  | 1:36:A:GLN:H    | 16       | 0.23          |
| (1,1113) | 1:35:A:GLN:HG3  | 1:36:A:GLN:H    | 16       | 0.23          |
| (1,1056) | 1:31:A:VAL:HG11 | 1:55:A:ARG:HA   | 9        | 0.23          |
| (1,1056) | 1:31:A:VAL:HG12 | 1:55:A:ARG:HA   | 9        | 0.23          |
| (1,1056) | 1:31:A:VAL:HG13 | 1:55:A:ARG:HA   | 9        | 0.23          |
| (1,1056) | 1:31:A:VAL:HG11 | 1:55:A:ARG:HA   | 14       | 0.23          |
| (1,1056) | 1:31:A:VAL:HG12 | 1:55:A:ARG:HA   | 14       | 0.23          |
| (1,1056) | 1:31:A:VAL:HG13 | 1:55:A:ARG:HA   | 14       | 0.23          |
| (1,1056) | 1:31:A:VAL:HG11 | 1:55:A:ARG:HA   | 17       | 0.23          |
| (1,1056) | 1:31:A:VAL:HG12 | 1:55:A:ARG:HA   | 17       | 0.23          |
| (1,1056) | 1:31:A:VAL:HG13 | 1:55:A:ARG:HA   | 17       | 0.23          |
| (1,961)  | 1:7:A:GLU:HA    | 1:7:A:GLU:HG2   | 9        | 0.23          |
| (1,924)  | 1:9:A:PRO:HD2   | 1:15:A:LEU:HB3  | 16       | 0.23          |
| (1,866)  | 1:65:A:LYS:HA   | 1:65:A:LYS:HG3  | 18       | 0.23          |
| (1,649)  | 1:52:A:ILE:HA   | 1:62:A:VAL:HG21 | 11       | 0.23          |
| (1,649)  | 1:52:A:ILE:HA   | 1:62:A:VAL:HG22 | 11       | 0.23          |
| (1,649)  | 1:52:A:ILE:HA   | 1:62:A:VAL:HG23 | 11       | 0.23          |
| (1,628)  | 1:34:A:LYS:H    | 1:34:A:LYS:HG2  | 19       | 0.23          |
| (1,430)  | 1:3:A:GLN:HA    | 1:3:A:GLN:HE22  | 3        | 0.23          |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD1  | 1        | 0.23          |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD2  | 1        | 0.23          |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD1  | 2        | 0.23          |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD2  | 2        | 0.23          |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD1  | 6        | 0.23          |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD2  | 6        | 0.23          |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD1  | 8        | 0.23          |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD2  | 8        | 0.23          |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD1  | 13       | 0.23          |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD2  | 13       | 0.23          |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD1  | 15       | 0.23          |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD2  | 15       | 0.23          |
| (1,340)  | 1:44:A:ASP:HB2  | 1:45:A:PHE:HD1  | 15       | 0.23          |
| (1,340)  | 1:44:A:ASP:HB2  | 1:45:A:PHE:HD2  | 15       | 0.23          |
| (1,340)  | 1:44:A:ASP:HB2  | 1:45:A:PHE:HD1  | 16       | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,340)  | 1:44:A:ASP:HB2  | 1:45:A:PHE:HD2  | 16       | 0.23          |
| (1,165)  | 1:35:A:GLN:H    | 1:35:A:GLN:HB2  | 20       | 0.23          |
| (1,126)  | 1:6:A:GLN:H     | 1:7:A:GLU:H     | 16       | 0.23          |
| (1,1253) | 1:32:A:TYR:HE1  | 1:62:A:VAL:HB   | 15       | 0.22          |
| (1,1253) | 1:32:A:TYR:HE2  | 1:62:A:VAL:HB   | 15       | 0.22          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB1  | 9        | 0.22          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB2  | 9        | 0.22          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB3  | 9        | 0.22          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB1  | 9        | 0.22          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB2  | 9        | 0.22          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB3  | 9        | 0.22          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB1  | 9        | 0.22          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB2  | 9        | 0.22          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB3  | 9        | 0.22          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB1  | 17       | 0.22          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB2  | 17       | 0.22          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB3  | 17       | 0.22          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB1  | 17       | 0.22          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB2  | 17       | 0.22          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB3  | 17       | 0.22          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB1  | 17       | 0.22          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB2  | 17       | 0.22          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB3  | 17       | 0.22          |
| (1,1244) | 1:30:A:CYS:H    | 1:63:A:CYS:H    | 9        | 0.22          |
| (1,1244) | 1:30:A:CYS:H    | 1:63:A:CYS:H    | 18       | 0.22          |
| (1,1242) | 1:29:A:GLU:HB2  | 1:60:A:TYR:HB2  | 6        | 0.22          |
| (1,1242) | 1:29:A:GLU:HB2  | 1:60:A:TYR:HB2  | 18       | 0.22          |
| (1,1242) | 1:29:A:GLU:HB2  | 1:60:A:TYR:HB2  | 20       | 0.22          |
| (1,1215) | 1:3:A:GLN:HE22  | 1:4:A:ASP:HA    | 20       | 0.22          |
| (1,1142) | 1:69:A:PHE:H    | 1:69:A:PHE:HB3  | 10       | 0.22          |
| (1,1057) | 1:1:A:MET:HE1   | 1:2:A:PHE:HA    | 18       | 0.22          |
| (1,1057) | 1:1:A:MET:HE2   | 1:2:A:PHE:HA    | 18       | 0.22          |
| (1,1057) | 1:1:A:MET:HE3   | 1:2:A:PHE:HA    | 18       | 0.22          |
| (1,1056) | 1:31:A:VAL:HG11 | 1:55:A:ARG:HA   | 1        | 0.22          |
| (1,1056) | 1:31:A:VAL:HG12 | 1:55:A:ARG:HA   | 1        | 0.22          |
| (1,1056) | 1:31:A:VAL:HG13 | 1:55:A:ARG:HA   | 1        | 0.22          |
| (1,924)  | 1:9:A:PRO:HD2   | 1:15:A:LEU:HB3  | 8        | 0.22          |
| (1,924)  | 1:9:A:PRO:HD2   | 1:15:A:LEU:HB3  | 18       | 0.22          |
| (1,649)  | 1:52:A:ILE:HA   | 1:62:A:VAL:HG21 | 5        | 0.22          |
| (1,649)  | 1:52:A:ILE:HA   | 1:62:A:VAL:HG22 | 5        | 0.22          |
| (1,649)  | 1:52:A:ILE:HA   | 1:62:A:VAL:HG23 | 5        | 0.22          |
| (1,649)  | 1:52:A:ILE:HA   | 1:62:A:VAL:HG21 | 12       | 0.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,649)  | 1:52:A:ILE:HA   | 1:62:A:VAL:HG22 | 12       | 0.22          |
| (1,649)  | 1:52:A:ILE:HA   | 1:62:A:VAL:HG23 | 12       | 0.22          |
| (1,625)  | 1:8:A:ARG:HG2   | 1:59:A:PRO:HG2  | 11       | 0.22          |
| (1,625)  | 1:8:A:ARG:HG3   | 1:59:A:PRO:HG2  | 11       | 0.22          |
| (1,554)  | 1:29:A:GLU:HG2  | 1:30:A:CYS:H    | 16       | 0.22          |
| (1,554)  | 1:29:A:GLU:HG3  | 1:30:A:CYS:H    | 16       | 0.22          |
| (1,430)  | 1:3:A:GLN:HA    | 1:3:A:GLN:HE22  | 12       | 0.22          |
| (1,430)  | 1:3:A:GLN:HA    | 1:3:A:GLN:HE22  | 18       | 0.22          |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD1  | 10       | 0.22          |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD2  | 10       | 0.22          |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD1  | 12       | 0.22          |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD2  | 12       | 0.22          |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD1  | 17       | 0.22          |
| (1,420)  | 1:29:A:GLU:HB3  | 1:60:A:TYR:HD2  | 17       | 0.22          |
| (1,401)  | 1:32:A:TYR:HD1  | 1:55:A:ARG:HG2  | 5        | 0.22          |
| (1,401)  | 1:32:A:TYR:HD2  | 1:55:A:ARG:HG2  | 5        | 0.22          |
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG11 | 7        | 0.22          |
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG12 | 7        | 0.22          |
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG13 | 7        | 0.22          |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG11 | 7        | 0.22          |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG12 | 7        | 0.22          |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG13 | 7        | 0.22          |
| (1,283)  | 1:23:A:ILE:HG12 | 1:24:A:HIS:HE1  | 10       | 0.22          |
| (1,97)   | 1:36:A:GLN:H    | 1:36:A:GLN:HB3  | 14       | 0.22          |
| (1,53)   | 1:37:A:LEU:H    | 1:37:A:LEU:HB3  | 9        | 0.22          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB1  | 2        | 0.21          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB2  | 2        | 0.21          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB3  | 2        | 0.21          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB1  | 2        | 0.21          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB2  | 2        | 0.21          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB3  | 2        | 0.21          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB1  | 2        | 0.21          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB2  | 2        | 0.21          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB3  | 2        | 0.21          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB1  | 5        | 0.21          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB2  | 5        | 0.21          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB3  | 5        | 0.21          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB1  | 5        | 0.21          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB2  | 5        | 0.21          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB3  | 5        | 0.21          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB1  | 5        | 0.21          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB2  | 5        | 0.21          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB3 | 5        | 0.21          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB1 | 11       | 0.21          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB2 | 11       | 0.21          |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB3 | 11       | 0.21          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB1 | 11       | 0.21          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB2 | 11       | 0.21          |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB3 | 11       | 0.21          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB1 | 11       | 0.21          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB2 | 11       | 0.21          |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB3 | 11       | 0.21          |
| (1,1244) | 1:30:A:CYS:H    | 1:63:A:CYS:H   | 20       | 0.21          |
| (1,1242) | 1:29:A:GLU:HB2  | 1:60:A:TYR:HB2 | 1        | 0.21          |
| (1,1242) | 1:29:A:GLU:HB2  | 1:60:A:TYR:HB2 | 9        | 0.21          |
| (1,1242) | 1:29:A:GLU:HB2  | 1:60:A:TYR:HB2 | 13       | 0.21          |
| (1,1242) | 1:29:A:GLU:HB2  | 1:60:A:TYR:HB2 | 14       | 0.21          |
| (1,1229) | 1:55:A:ARG:HG3  | 1:32:A:TYR:H   | 4        | 0.21          |
| (1,1229) | 1:55:A:ARG:HG3  | 1:32:A:TYR:H   | 8        | 0.21          |
| (1,1229) | 1:55:A:ARG:HG3  | 1:32:A:TYR:H   | 11       | 0.21          |
| (1,1229) | 1:55:A:ARG:HG3  | 1:32:A:TYR:H   | 18       | 0.21          |
| (1,1229) | 1:55:A:ARG:HG3  | 1:32:A:TYR:H   | 20       | 0.21          |
| (1,1215) | 1:3:A:GLN:HE22  | 1:4:A:ASP:HA   | 4        | 0.21          |
| (1,1215) | 1:3:A:GLN:HE22  | 1:4:A:ASP:HA   | 14       | 0.21          |
| (1,1142) | 1:69:A:PHE:H    | 1:69:A:PHE:HB3 | 3        | 0.21          |
| (1,1142) | 1:69:A:PHE:H    | 1:69:A:PHE:HB3 | 15       | 0.21          |
| (1,1142) | 1:69:A:PHE:H    | 1:69:A:PHE:HB3 | 17       | 0.21          |
| (1,1072) | 1:29:A:GLU:HB2  | 1:37:A:LEU:H   | 16       | 0.21          |
| (1,1056) | 1:31:A:VAL:HG11 | 1:55:A:ARG:HA  | 7        | 0.21          |
| (1,1056) | 1:31:A:VAL:HG12 | 1:55:A:ARG:HA  | 7        | 0.21          |
| (1,1056) | 1:31:A:VAL:HG13 | 1:55:A:ARG:HA  | 7        | 0.21          |
| (1,1056) | 1:31:A:VAL:HG11 | 1:55:A:ARG:HA  | 13       | 0.21          |
| (1,1056) | 1:31:A:VAL:HG12 | 1:55:A:ARG:HA  | 13       | 0.21          |
| (1,1056) | 1:31:A:VAL:HG13 | 1:55:A:ARG:HA  | 13       | 0.21          |
| (1,1056) | 1:31:A:VAL:HG11 | 1:55:A:ARG:HA  | 15       | 0.21          |
| (1,1056) | 1:31:A:VAL:HG12 | 1:55:A:ARG:HA  | 15       | 0.21          |
| (1,1056) | 1:31:A:VAL:HG13 | 1:55:A:ARG:HA  | 15       | 0.21          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB1 | 3        | 0.21          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB2 | 3        | 0.21          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB3 | 3        | 0.21          |
| (1,924)  | 1:9:A:PRO:HD2   | 1:15:A:LEU:HB3 | 12       | 0.21          |
| (1,905)  | 1:77:A:ARG:HA   | 1:77:A:ARG:HD2 | 18       | 0.21          |
| (1,905)  | 1:77:A:ARG:HA   | 1:77:A:ARG:HD3 | 18       | 0.21          |
| (1,866)  | 1:65:A:LYS:HA   | 1:65:A:LYS:HG3 | 16       | 0.21          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,760) | 1:48:A:ARG:HD3 | 1:50:A:LEU:HD21 | 13       | 0.21          |
| (1,760) | 1:48:A:ARG:HD3 | 1:50:A:LEU:HD22 | 13       | 0.21          |
| (1,760) | 1:48:A:ARG:HD3 | 1:50:A:LEU:HD23 | 13       | 0.21          |
| (1,649) | 1:52:A:ILE:HA  | 1:62:A:VAL:HG21 | 7        | 0.21          |
| (1,649) | 1:52:A:ILE:HA  | 1:62:A:VAL:HG22 | 7        | 0.21          |
| (1,649) | 1:52:A:ILE:HA  | 1:62:A:VAL:HG23 | 7        | 0.21          |
| (1,649) | 1:52:A:ILE:HA  | 1:62:A:VAL:HG21 | 10       | 0.21          |
| (1,649) | 1:52:A:ILE:HA  | 1:62:A:VAL:HG22 | 10       | 0.21          |
| (1,649) | 1:52:A:ILE:HA  | 1:62:A:VAL:HG23 | 10       | 0.21          |
| (1,649) | 1:52:A:ILE:HA  | 1:62:A:VAL:HG21 | 14       | 0.21          |
| (1,649) | 1:52:A:ILE:HA  | 1:62:A:VAL:HG22 | 14       | 0.21          |
| (1,649) | 1:52:A:ILE:HA  | 1:62:A:VAL:HG23 | 14       | 0.21          |
| (1,649) | 1:52:A:ILE:HA  | 1:62:A:VAL:HG21 | 17       | 0.21          |
| (1,649) | 1:52:A:ILE:HA  | 1:62:A:VAL:HG22 | 17       | 0.21          |
| (1,649) | 1:52:A:ILE:HA  | 1:62:A:VAL:HG23 | 17       | 0.21          |
| (1,628) | 1:34:A:LYS:H   | 1:34:A:LYS:HG2  | 3        | 0.21          |
| (1,628) | 1:34:A:LYS:H   | 1:34:A:LYS:HG2  | 11       | 0.21          |
| (1,628) | 1:34:A:LYS:H   | 1:34:A:LYS:HG2  | 17       | 0.21          |
| (1,556) | 1:29:A:GLU:HG2 | 1:60:A:TYR:HB2  | 7        | 0.21          |
| (1,556) | 1:29:A:GLU:HG3 | 1:60:A:TYR:HB2  | 7        | 0.21          |
| (1,420) | 1:29:A:GLU:HB3 | 1:60:A:TYR:HD1  | 3        | 0.21          |
| (1,420) | 1:29:A:GLU:HB3 | 1:60:A:TYR:HD2  | 3        | 0.21          |
| (1,420) | 1:29:A:GLU:HB3 | 1:60:A:TYR:HD1  | 4        | 0.21          |
| (1,420) | 1:29:A:GLU:HB3 | 1:60:A:TYR:HD2  | 4        | 0.21          |
| (1,420) | 1:29:A:GLU:HB3 | 1:60:A:TYR:HD1  | 9        | 0.21          |
| (1,420) | 1:29:A:GLU:HB3 | 1:60:A:TYR:HD2  | 9        | 0.21          |
| (1,420) | 1:29:A:GLU:HB3 | 1:60:A:TYR:HD1  | 11       | 0.21          |
| (1,420) | 1:29:A:GLU:HB3 | 1:60:A:TYR:HD2  | 11       | 0.21          |
| (1,420) | 1:29:A:GLU:HB3 | 1:60:A:TYR:HD1  | 14       | 0.21          |
| (1,420) | 1:29:A:GLU:HB3 | 1:60:A:TYR:HD2  | 14       | 0.21          |
| (1,401) | 1:32:A:TYR:HD1 | 1:55:A:ARG:HG2  | 13       | 0.21          |
| (1,401) | 1:32:A:TYR:HD2 | 1:55:A:ARG:HG2  | 13       | 0.21          |
| (1,340) | 1:44:A:ASP:HB2 | 1:45:A:PHE:HD1  | 7        | 0.21          |
| (1,340) | 1:44:A:ASP:HB2 | 1:45:A:PHE:HD2  | 7        | 0.21          |
| (1,340) | 1:44:A:ASP:HB2 | 1:45:A:PHE:HD1  | 9        | 0.21          |
| (1,340) | 1:44:A:ASP:HB2 | 1:45:A:PHE:HD2  | 9        | 0.21          |
| (1,340) | 1:44:A:ASP:HB2 | 1:45:A:PHE:HD1  | 17       | 0.21          |
| (1,340) | 1:44:A:ASP:HB2 | 1:45:A:PHE:HD2  | 17       | 0.21          |
| (1,334) | 1:45:A:PHE:HD1 | 1:62:A:VAL:HG11 | 6        | 0.21          |
| (1,334) | 1:45:A:PHE:HD1 | 1:62:A:VAL:HG12 | 6        | 0.21          |
| (1,334) | 1:45:A:PHE:HD1 | 1:62:A:VAL:HG13 | 6        | 0.21          |
| (1,334) | 1:45:A:PHE:HD2 | 1:62:A:VAL:HG11 | 6        | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG12 | 6        | 0.21          |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG13 | 6        | 0.21          |
| (1,321)  | 1:2:A:PHE:HD1   | 1:19:A:LEU:HG   | 14       | 0.21          |
| (1,321)  | 1:2:A:PHE:HD2   | 1:19:A:LEU:HG   | 14       | 0.21          |
| (1,310)  | 1:2:A:PHE:HD1   | 1:8:A:ARG:H     | 15       | 0.21          |
| (1,310)  | 1:2:A:PHE:HD2   | 1:8:A:ARG:H     | 15       | 0.21          |
| (1,283)  | 1:23:A:ILE:HG12 | 1:24:A:HIS:HE1  | 20       | 0.21          |
| (1,165)  | 1:35:A:GLN:H    | 1:35:A:GLN:HB2  | 5        | 0.21          |
| (1,126)  | 1:6:A:GLN:H     | 1:7:A:GLU:H     | 19       | 0.21          |
| (1,97)   | 1:36:A:GLN:H    | 1:36:A:GLN:HB3  | 4        | 0.21          |
| (1,53)   | 1:37:A:LEU:H    | 1:37:A:LEU:HB3  | 4        | 0.21          |
| (1,53)   | 1:37:A:LEU:H    | 1:37:A:LEU:HB3  | 16       | 0.21          |
| (1,53)   | 1:37:A:LEU:H    | 1:37:A:LEU:HB3  | 18       | 0.21          |
| (1,1253) | 1:32:A:TYR:HE1  | 1:62:A:VAL:HB   | 3        | 0.2           |
| (1,1253) | 1:32:A:TYR:HE2  | 1:62:A:VAL:HB   | 3        | 0.2           |
| (1,1253) | 1:32:A:TYR:HE1  | 1:62:A:VAL:HB   | 5        | 0.2           |
| (1,1253) | 1:32:A:TYR:HE2  | 1:62:A:VAL:HB   | 5        | 0.2           |
| (1,1253) | 1:32:A:TYR:HE1  | 1:62:A:VAL:HB   | 17       | 0.2           |
| (1,1253) | 1:32:A:TYR:HE2  | 1:62:A:VAL:HB   | 17       | 0.2           |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB1  | 8        | 0.2           |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB2  | 8        | 0.2           |
| (1,1250) | 1:31:A:VAL:HG11 | 1:61:A:ALA:HB3  | 8        | 0.2           |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB1  | 8        | 0.2           |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB2  | 8        | 0.2           |
| (1,1250) | 1:31:A:VAL:HG12 | 1:61:A:ALA:HB3  | 8        | 0.2           |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB1  | 8        | 0.2           |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB2  | 8        | 0.2           |
| (1,1250) | 1:31:A:VAL:HG13 | 1:61:A:ALA:HB3  | 8        | 0.2           |
| (1,1244) | 1:30:A:CYS:H    | 1:63:A:CYS:H    | 17       | 0.2           |
| (1,1242) | 1:29:A:GLU:HB2  | 1:60:A:TYR:HB2  | 10       | 0.2           |
| (1,1229) | 1:55:A:ARG:HG3  | 1:32:A:TYR:H    | 17       | 0.2           |
| (1,1142) | 1:69:A:PHE:H    | 1:69:A:PHE:HB3  | 8        | 0.2           |
| (1,1142) | 1:69:A:PHE:H    | 1:69:A:PHE:HB3  | 16       | 0.2           |
| (1,1118) | 1:7:A:GLU:HA    | 1:8:A:ARG:H     | 19       | 0.2           |
| (1,1114) | 1:36:A:GLN:H    | 1:36:A:GLN:HG3  | 15       | 0.2           |
| (1,1098) | 1:77:A:ARG:H    | 1:78:A:HIS:HD2  | 18       | 0.2           |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB1  | 11       | 0.2           |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB2  | 11       | 0.2           |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB3  | 11       | 0.2           |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB1  | 12       | 0.2           |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB2  | 12       | 0.2           |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB3  | 12       | 0.2           |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1042) | 1:28:A:LEU:HA  | 1:61:A:ALA:HB1  | 17       | 0.2           |
| (1,1042) | 1:28:A:LEU:HA  | 1:61:A:ALA:HB2  | 17       | 0.2           |
| (1,1042) | 1:28:A:LEU:HA  | 1:61:A:ALA:HB3  | 17       | 0.2           |
| (1,968)  | 1:35:A:GLN:H   | 1:35:A:GLN:HG2  | 15       | 0.2           |
| (1,968)  | 1:35:A:GLN:H   | 1:35:A:GLN:HG3  | 15       | 0.2           |
| (1,961)  | 1:7:A:GLU:HA   | 1:7:A:GLU:HG2   | 16       | 0.2           |
| (1,958)  | 1:29:A:GLU:HA  | 1:29:A:GLU:HG2  | 8        | 0.2           |
| (1,958)  | 1:29:A:GLU:HA  | 1:29:A:GLU:HG3  | 8        | 0.2           |
| (1,958)  | 1:29:A:GLU:HA  | 1:29:A:GLU:HG2  | 14       | 0.2           |
| (1,958)  | 1:29:A:GLU:HA  | 1:29:A:GLU:HG3  | 14       | 0.2           |
| (1,866)  | 1:65:A:LYS:HA  | 1:65:A:LYS:HG3  | 14       | 0.2           |
| (1,760)  | 1:48:A:ARG:HD3 | 1:50:A:LEU:HD21 | 7        | 0.2           |
| (1,760)  | 1:48:A:ARG:HD3 | 1:50:A:LEU:HD22 | 7        | 0.2           |
| (1,760)  | 1:48:A:ARG:HD3 | 1:50:A:LEU:HD23 | 7        | 0.2           |
| (1,689)  | 1:67:A:LEU:HA  | 1:67:A:LEU:HD11 | 17       | 0.2           |
| (1,689)  | 1:67:A:LEU:HA  | 1:67:A:LEU:HD12 | 17       | 0.2           |
| (1,689)  | 1:67:A:LEU:HA  | 1:67:A:LEU:HD13 | 17       | 0.2           |
| (1,649)  | 1:52:A:ILE:HA  | 1:62:A:VAL:HG21 | 3        | 0.2           |
| (1,649)  | 1:52:A:ILE:HA  | 1:62:A:VAL:HG22 | 3        | 0.2           |
| (1,649)  | 1:52:A:ILE:HA  | 1:62:A:VAL:HG23 | 3        | 0.2           |
| (1,649)  | 1:52:A:ILE:HA  | 1:62:A:VAL:HG21 | 4        | 0.2           |
| (1,649)  | 1:52:A:ILE:HA  | 1:62:A:VAL:HG22 | 4        | 0.2           |
| (1,649)  | 1:52:A:ILE:HA  | 1:62:A:VAL:HG23 | 4        | 0.2           |
| (1,649)  | 1:52:A:ILE:HA  | 1:62:A:VAL:HG21 | 6        | 0.2           |
| (1,649)  | 1:52:A:ILE:HA  | 1:62:A:VAL:HG22 | 6        | 0.2           |
| (1,649)  | 1:52:A:ILE:HA  | 1:62:A:VAL:HG23 | 6        | 0.2           |
| (1,649)  | 1:52:A:ILE:HA  | 1:62:A:VAL:HG21 | 18       | 0.2           |
| (1,649)  | 1:52:A:ILE:HA  | 1:62:A:VAL:HG22 | 18       | 0.2           |
| (1,649)  | 1:52:A:ILE:HA  | 1:62:A:VAL:HG23 | 18       | 0.2           |
| (1,625)  | 1:8:A:ARG:HG2  | 1:59:A:PRO:HG2  | 2        | 0.2           |
| (1,625)  | 1:8:A:ARG:HG3  | 1:59:A:PRO:HG2  | 2        | 0.2           |
| (1,455)  | 1:54:A:TYR:HD1 | 1:59:A:PRO:HB2  | 11       | 0.2           |
| (1,455)  | 1:54:A:TYR:HD2 | 1:59:A:PRO:HB2  | 11       | 0.2           |
| (1,430)  | 1:3:A:GLN:HA   | 1:3:A:GLN:HE22  | 7        | 0.2           |
| (1,340)  | 1:44:A:ASP:HB2 | 1:45:A:PHE:HD1  | 1        | 0.2           |
| (1,340)  | 1:44:A:ASP:HB2 | 1:45:A:PHE:HD2  | 1        | 0.2           |
| (1,340)  | 1:44:A:ASP:HB2 | 1:45:A:PHE:HD1  | 4        | 0.2           |
| (1,340)  | 1:44:A:ASP:HB2 | 1:45:A:PHE:HD2  | 4        | 0.2           |
| (1,340)  | 1:44:A:ASP:HB2 | 1:45:A:PHE:HD1  | 10       | 0.2           |
| (1,340)  | 1:44:A:ASP:HB2 | 1:45:A:PHE:HD2  | 10       | 0.2           |
| (1,340)  | 1:44:A:ASP:HB2 | 1:45:A:PHE:HD1  | 20       | 0.2           |
| (1,340)  | 1:44:A:ASP:HB2 | 1:45:A:PHE:HD2  | 20       | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG11 | 3        | 0.2           |
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG12 | 3        | 0.2           |
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG13 | 3        | 0.2           |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG11 | 3        | 0.2           |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG12 | 3        | 0.2           |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG13 | 3        | 0.2           |
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG11 | 11       | 0.2           |
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG12 | 11       | 0.2           |
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG13 | 11       | 0.2           |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG11 | 11       | 0.2           |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG12 | 11       | 0.2           |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG13 | 11       | 0.2           |
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG11 | 16       | 0.2           |
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG12 | 16       | 0.2           |
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG13 | 16       | 0.2           |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG11 | 16       | 0.2           |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG12 | 16       | 0.2           |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG13 | 16       | 0.2           |
| (1,313)  | 1:2:A:PHE:H     | 1:2:A:PHE:HD1   | 19       | 0.2           |
| (1,313)  | 1:2:A:PHE:H     | 1:2:A:PHE:HD2   | 19       | 0.2           |
| (1,283)  | 1:23:A:ILE:HG12 | 1:24:A:HIS:HE1  | 1        | 0.2           |
| (1,283)  | 1:23:A:ILE:HG12 | 1:24:A:HIS:HE1  | 6        | 0.2           |
| (1,283)  | 1:23:A:ILE:HG12 | 1:24:A:HIS:HE1  | 9        | 0.2           |
| (1,283)  | 1:23:A:ILE:HG12 | 1:24:A:HIS:HE1  | 15       | 0.2           |
| (1,283)  | 1:23:A:ILE:HG12 | 1:24:A:HIS:HE1  | 16       | 0.2           |
| (1,283)  | 1:23:A:ILE:HG12 | 1:24:A:HIS:HE1  | 17       | 0.2           |
| (1,283)  | 1:23:A:ILE:HG12 | 1:24:A:HIS:HE1  | 18       | 0.2           |
| (1,241)  | 1:34:A:LYS:H    | 1:34:A:LYS:HG3  | 1        | 0.2           |
| (1,165)  | 1:35:A:GLN:H    | 1:35:A:GLN:HB2  | 10       | 0.2           |
| (1,165)  | 1:35:A:GLN:H    | 1:35:A:GLN:HB2  | 12       | 0.2           |
| (1,165)  | 1:35:A:GLN:H    | 1:35:A:GLN:HB2  | 13       | 0.2           |
| (1,126)  | 1:6:A:GLN:H     | 1:7:A:GLU:H     | 9        | 0.2           |
| (1,97)   | 1:36:A:GLN:H    | 1:36:A:GLN:HB3  | 6        | 0.2           |
| (1,97)   | 1:36:A:GLN:H    | 1:36:A:GLN:HB3  | 7        | 0.2           |
| (1,97)   | 1:36:A:GLN:H    | 1:36:A:GLN:HB3  | 12       | 0.2           |
| (1,97)   | 1:36:A:GLN:H    | 1:36:A:GLN:HB3  | 18       | 0.2           |
| (1,53)   | 1:37:A:LEU:H    | 1:37:A:LEU:HB3  | 11       | 0.2           |
| (1,1253) | 1:32:A:TYR:HE1  | 1:62:A:VAL:HB   | 2        | 0.19          |
| (1,1253) | 1:32:A:TYR:HE2  | 1:62:A:VAL:HB   | 2        | 0.19          |
| (1,1253) | 1:32:A:TYR:HE1  | 1:62:A:VAL:HB   | 7        | 0.19          |
| (1,1253) | 1:32:A:TYR:HE2  | 1:62:A:VAL:HB   | 7        | 0.19          |
| (1,1253) | 1:32:A:TYR:HE1  | 1:62:A:VAL:HB   | 18       | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1253) | 1:32:A:TYR:HE2  | 1:62:A:VAL:HB   | 18       | 0.19          |
| (1,1244) | 1:30:A:CYS:H    | 1:63:A:CYS:H    | 2        | 0.19          |
| (1,1244) | 1:30:A:CYS:H    | 1:63:A:CYS:H    | 3        | 0.19          |
| (1,1244) | 1:30:A:CYS:H    | 1:63:A:CYS:H    | 10       | 0.19          |
| (1,1242) | 1:29:A:GLU:HB2  | 1:60:A:TYR:HB2  | 3        | 0.19          |
| (1,1242) | 1:29:A:GLU:HB2  | 1:60:A:TYR:HB2  | 17       | 0.19          |
| (1,1229) | 1:55:A:ARG:HG3  | 1:32:A:TYR:H    | 2        | 0.19          |
| (1,1229) | 1:55:A:ARG:HG3  | 1:32:A:TYR:H    | 10       | 0.19          |
| (1,1229) | 1:55:A:ARG:HG3  | 1:32:A:TYR:H    | 14       | 0.19          |
| (1,1229) | 1:55:A:ARG:HG3  | 1:32:A:TYR:H    | 19       | 0.19          |
| (1,1215) | 1:3:A:GLN:HE22  | 1:4:A:ASP:HA    | 15       | 0.19          |
| (1,1133) | 1:65:A:LYS:H    | 1:65:A:LYS:HD2  | 6        | 0.19          |
| (1,1133) | 1:65:A:LYS:H    | 1:65:A:LYS:HD3  | 6        | 0.19          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB1  | 6        | 0.19          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB2  | 6        | 0.19          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB3  | 6        | 0.19          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB1  | 14       | 0.19          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB2  | 14       | 0.19          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB3  | 14       | 0.19          |
| (1,996)  | 1:10:A:ARG:HA   | 1:10:A:ARG:HG2  | 4        | 0.19          |
| (1,996)  | 1:10:A:ARG:HA   | 1:10:A:ARG:HG2  | 9        | 0.19          |
| (1,968)  | 1:35:A:GLN:H    | 1:35:A:GLN:HG2  | 18       | 0.19          |
| (1,968)  | 1:35:A:GLN:H    | 1:35:A:GLN:HG3  | 18       | 0.19          |
| (1,958)  | 1:29:A:GLU:HA   | 1:29:A:GLU:HG2  | 3        | 0.19          |
| (1,958)  | 1:29:A:GLU:HA   | 1:29:A:GLU:HG3  | 3        | 0.19          |
| (1,958)  | 1:29:A:GLU:HA   | 1:29:A:GLU:HG2  | 9        | 0.19          |
| (1,958)  | 1:29:A:GLU:HA   | 1:29:A:GLU:HG3  | 9        | 0.19          |
| (1,958)  | 1:29:A:GLU:HA   | 1:29:A:GLU:HG2  | 12       | 0.19          |
| (1,958)  | 1:29:A:GLU:HA   | 1:29:A:GLU:HG3  | 12       | 0.19          |
| (1,958)  | 1:29:A:GLU:HA   | 1:29:A:GLU:HG2  | 15       | 0.19          |
| (1,958)  | 1:29:A:GLU:HA   | 1:29:A:GLU:HG3  | 15       | 0.19          |
| (1,932)  | 1:10:A:ARG:HA   | 1:10:A:ARG:HD2  | 8        | 0.19          |
| (1,932)  | 1:10:A:ARG:HA   | 1:10:A:ARG:HD3  | 8        | 0.19          |
| (1,866)  | 1:65:A:LYS:HA   | 1:65:A:LYS:HG3  | 12       | 0.19          |
| (1,776)  | 1:52:A:ILE:HA   | 1:52:A:ILE:HD11 | 4        | 0.19          |
| (1,776)  | 1:52:A:ILE:HA   | 1:52:A:ILE:HD12 | 4        | 0.19          |
| (1,776)  | 1:52:A:ILE:HA   | 1:52:A:ILE:HD13 | 4        | 0.19          |
| (1,776)  | 1:52:A:ILE:HA   | 1:52:A:ILE:HD11 | 8        | 0.19          |
| (1,776)  | 1:52:A:ILE:HA   | 1:52:A:ILE:HD12 | 8        | 0.19          |
| (1,776)  | 1:52:A:ILE:HA   | 1:52:A:ILE:HD13 | 8        | 0.19          |
| (1,717)  | 1:53:A:VAL:HG11 | 1:60:A:TYR:HB3  | 18       | 0.19          |
| (1,717)  | 1:53:A:VAL:HG12 | 1:60:A:TYR:HB3  | 18       | 0.19          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,717) | 1:53:A:VAL:HG13 | 1:60:A:TYR:HB3  | 18       | 0.19          |
| (1,717) | 1:53:A:VAL:HG21 | 1:60:A:TYR:HB3  | 18       | 0.19          |
| (1,717) | 1:53:A:VAL:HG22 | 1:60:A:TYR:HB3  | 18       | 0.19          |
| (1,717) | 1:53:A:VAL:HG23 | 1:60:A:TYR:HB3  | 18       | 0.19          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD21 | 2        | 0.19          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD22 | 2        | 0.19          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD23 | 2        | 0.19          |
| (1,691) | 1:18:A:GLU:HG3  | 1:19:A:LEU:HD11 | 14       | 0.19          |
| (1,691) | 1:18:A:GLU:HG3  | 1:19:A:LEU:HD12 | 14       | 0.19          |
| (1,691) | 1:18:A:GLU:HG3  | 1:19:A:LEU:HD13 | 14       | 0.19          |
| (1,649) | 1:52:A:ILE:HA   | 1:62:A:VAL:HG21 | 15       | 0.19          |
| (1,649) | 1:52:A:ILE:HA   | 1:62:A:VAL:HG22 | 15       | 0.19          |
| (1,649) | 1:52:A:ILE:HA   | 1:62:A:VAL:HG23 | 15       | 0.19          |
| (1,649) | 1:52:A:ILE:HA   | 1:62:A:VAL:HG21 | 19       | 0.19          |
| (1,649) | 1:52:A:ILE:HA   | 1:62:A:VAL:HG22 | 19       | 0.19          |
| (1,649) | 1:52:A:ILE:HA   | 1:62:A:VAL:HG23 | 19       | 0.19          |
| (1,649) | 1:52:A:ILE:HA   | 1:62:A:VAL:HG21 | 20       | 0.19          |
| (1,649) | 1:52:A:ILE:HA   | 1:62:A:VAL:HG22 | 20       | 0.19          |
| (1,649) | 1:52:A:ILE:HA   | 1:62:A:VAL:HG23 | 20       | 0.19          |
| (1,574) | 1:11:A:LYS:HA   | 1:11:A:LYS:HD2  | 17       | 0.19          |
| (1,574) | 1:11:A:LYS:HA   | 1:11:A:LYS:HD3  | 17       | 0.19          |
| (1,465) | 1:32:A:TYR:HE1  | 1:55:A:ARG:HG2  | 9        | 0.19          |
| (1,465) | 1:32:A:TYR:HE2  | 1:55:A:ARG:HG2  | 9        | 0.19          |
| (1,430) | 1:3:A:GLN:HA    | 1:3:A:GLN:HE22  | 19       | 0.19          |
| (1,409) | 1:78:A:HIS:HB2  | 1:78:A:HIS:HD2  | 6        | 0.19          |
| (1,409) | 1:78:A:HIS:HB2  | 1:78:A:HIS:HD2  | 14       | 0.19          |
| (1,382) | 1:78:A:HIS:HB3  | 1:79:A:TYR:HD1  | 17       | 0.19          |
| (1,382) | 1:78:A:HIS:HB3  | 1:79:A:TYR:HD2  | 17       | 0.19          |
| (1,340) | 1:44:A:ASP:HB2  | 1:45:A:PHE:HD1  | 3        | 0.19          |
| (1,340) | 1:44:A:ASP:HB2  | 1:45:A:PHE:HD2  | 3        | 0.19          |
| (1,340) | 1:44:A:ASP:HB2  | 1:45:A:PHE:HD1  | 5        | 0.19          |
| (1,340) | 1:44:A:ASP:HB2  | 1:45:A:PHE:HD2  | 5        | 0.19          |
| (1,340) | 1:44:A:ASP:HB2  | 1:45:A:PHE:HD1  | 18       | 0.19          |
| (1,340) | 1:44:A:ASP:HB2  | 1:45:A:PHE:HD2  | 18       | 0.19          |
| (1,340) | 1:44:A:ASP:HB2  | 1:45:A:PHE:HD1  | 19       | 0.19          |
| (1,340) | 1:44:A:ASP:HB2  | 1:45:A:PHE:HD2  | 19       | 0.19          |
| (1,334) | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG11 | 17       | 0.19          |
| (1,334) | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG12 | 17       | 0.19          |
| (1,334) | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG13 | 17       | 0.19          |
| (1,334) | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG11 | 17       | 0.19          |
| (1,334) | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG12 | 17       | 0.19          |
| (1,334) | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG13 | 17       | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG11 | 20       | 0.19          |
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG12 | 20       | 0.19          |
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG13 | 20       | 0.19          |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG11 | 20       | 0.19          |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG12 | 20       | 0.19          |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG13 | 20       | 0.19          |
| (1,283)  | 1:23:A:ILE:HG12 | 1:24:A:HIS:HE1  | 3        | 0.19          |
| (1,283)  | 1:23:A:ILE:HG12 | 1:24:A:HIS:HE1  | 5        | 0.19          |
| (1,283)  | 1:23:A:ILE:HG12 | 1:24:A:HIS:HE1  | 7        | 0.19          |
| (1,283)  | 1:23:A:ILE:HG12 | 1:24:A:HIS:HE1  | 8        | 0.19          |
| (1,283)  | 1:23:A:ILE:HG12 | 1:24:A:HIS:HE1  | 12       | 0.19          |
| (1,283)  | 1:23:A:ILE:HG12 | 1:24:A:HIS:HE1  | 14       | 0.19          |
| (1,283)  | 1:23:A:ILE:HG12 | 1:24:A:HIS:HE1  | 19       | 0.19          |
| (1,241)  | 1:34:A:LYS:H    | 1:34:A:LYS:HG3  | 4        | 0.19          |
| (1,165)  | 1:35:A:GLN:H    | 1:35:A:GLN:HB2  | 4        | 0.19          |
| (1,82)   | 1:54:A:TYR:H    | 1:59:A:PRO:HA   | 14       | 0.19          |
| (1,53)   | 1:37:A:LEU:H    | 1:37:A:LEU:HB3  | 2        | 0.19          |
| (1,53)   | 1:37:A:LEU:H    | 1:37:A:LEU:HB3  | 14       | 0.19          |
| (1,1253) | 1:32:A:TYR:HE1  | 1:62:A:VAL:HB   | 6        | 0.18          |
| (1,1253) | 1:32:A:TYR:HE2  | 1:62:A:VAL:HB   | 6        | 0.18          |
| (1,1253) | 1:32:A:TYR:HE1  | 1:62:A:VAL:HB   | 8        | 0.18          |
| (1,1253) | 1:32:A:TYR:HE2  | 1:62:A:VAL:HB   | 8        | 0.18          |
| (1,1253) | 1:32:A:TYR:HE1  | 1:62:A:VAL:HB   | 10       | 0.18          |
| (1,1253) | 1:32:A:TYR:HE2  | 1:62:A:VAL:HB   | 10       | 0.18          |
| (1,1253) | 1:32:A:TYR:HE1  | 1:62:A:VAL:HB   | 12       | 0.18          |
| (1,1253) | 1:32:A:TYR:HE2  | 1:62:A:VAL:HB   | 12       | 0.18          |
| (1,1244) | 1:30:A:CYS:H    | 1:63:A:CYS:H    | 1        | 0.18          |
| (1,1244) | 1:30:A:CYS:H    | 1:63:A:CYS:H    | 6        | 0.18          |
| (1,1244) | 1:30:A:CYS:H    | 1:63:A:CYS:H    | 11       | 0.18          |
| (1,1242) | 1:29:A:GLU:HB2  | 1:60:A:TYR:HB2  | 7        | 0.18          |
| (1,1242) | 1:29:A:GLU:HB2  | 1:60:A:TYR:HB2  | 11       | 0.18          |
| (1,1242) | 1:29:A:GLU:HB2  | 1:60:A:TYR:HB2  | 19       | 0.18          |
| (1,1234) | 1:10:A:ARG:HA   | 1:52:A:ILE:HD11 | 10       | 0.18          |
| (1,1234) | 1:10:A:ARG:HA   | 1:52:A:ILE:HD12 | 10       | 0.18          |
| (1,1234) | 1:10:A:ARG:HA   | 1:52:A:ILE:HD13 | 10       | 0.18          |
| (1,1234) | 1:10:A:ARG:HA   | 1:52:A:ILE:HD11 | 14       | 0.18          |
| (1,1234) | 1:10:A:ARG:HA   | 1:52:A:ILE:HD12 | 14       | 0.18          |
| (1,1234) | 1:10:A:ARG:HA   | 1:52:A:ILE:HD13 | 14       | 0.18          |
| (1,1228) | 1:9:A:PRO:HG2   | 1:54:A:TYR:HE1  | 11       | 0.18          |
| (1,1228) | 1:9:A:PRO:HG2   | 1:54:A:TYR:HE2  | 11       | 0.18          |
| (1,1228) | 1:9:A:PRO:HG3   | 1:54:A:TYR:HE1  | 11       | 0.18          |
| (1,1228) | 1:9:A:PRO:HG3   | 1:54:A:TYR:HE2  | 11       | 0.18          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1142) | 1:69:A:PHE:H   | 1:69:A:PHE:HB3  | 4        | 0.18          |
| (1,1142) | 1:69:A:PHE:H   | 1:69:A:PHE:HB3  | 13       | 0.18          |
| (1,1118) | 1:7:A:GLU:HA   | 1:8:A:ARG:H     | 9        | 0.18          |
| (1,1114) | 1:36:A:GLN:H   | 1:36:A:GLN:HG3  | 3        | 0.18          |
| (1,1042) | 1:28:A:LEU:HA  | 1:61:A:ALA:HB1  | 4        | 0.18          |
| (1,1042) | 1:28:A:LEU:HA  | 1:61:A:ALA:HB2  | 4        | 0.18          |
| (1,1042) | 1:28:A:LEU:HA  | 1:61:A:ALA:HB3  | 4        | 0.18          |
| (1,1042) | 1:28:A:LEU:HA  | 1:61:A:ALA:HB1  | 8        | 0.18          |
| (1,1042) | 1:28:A:LEU:HA  | 1:61:A:ALA:HB2  | 8        | 0.18          |
| (1,1042) | 1:28:A:LEU:HA  | 1:61:A:ALA:HB3  | 8        | 0.18          |
| (1,1042) | 1:28:A:LEU:HA  | 1:61:A:ALA:HB1  | 9        | 0.18          |
| (1,1042) | 1:28:A:LEU:HA  | 1:61:A:ALA:HB2  | 9        | 0.18          |
| (1,1042) | 1:28:A:LEU:HA  | 1:61:A:ALA:HB3  | 9        | 0.18          |
| (1,1042) | 1:28:A:LEU:HA  | 1:61:A:ALA:HB1  | 10       | 0.18          |
| (1,1042) | 1:28:A:LEU:HA  | 1:61:A:ALA:HB2  | 10       | 0.18          |
| (1,1042) | 1:28:A:LEU:HA  | 1:61:A:ALA:HB3  | 10       | 0.18          |
| (1,1042) | 1:28:A:LEU:HA  | 1:61:A:ALA:HB1  | 19       | 0.18          |
| (1,1042) | 1:28:A:LEU:HA  | 1:61:A:ALA:HB2  | 19       | 0.18          |
| (1,1042) | 1:28:A:LEU:HA  | 1:61:A:ALA:HB3  | 19       | 0.18          |
| (1,1042) | 1:28:A:LEU:HA  | 1:61:A:ALA:HB1  | 20       | 0.18          |
| (1,1042) | 1:28:A:LEU:HA  | 1:61:A:ALA:HB2  | 20       | 0.18          |
| (1,1042) | 1:28:A:LEU:HA  | 1:61:A:ALA:HB3  | 20       | 0.18          |
| (1,966)  | 1:33:A:CYS:HB2 | 1:35:A:GLN:HG2  | 20       | 0.18          |
| (1,966)  | 1:33:A:CYS:HB2 | 1:35:A:GLN:HG3  | 20       | 0.18          |
| (1,958)  | 1:29:A:GLU:HA  | 1:29:A:GLU:HG2  | 2        | 0.18          |
| (1,958)  | 1:29:A:GLU:HA  | 1:29:A:GLU:HG3  | 2        | 0.18          |
| (1,932)  | 1:10:A:ARG:HA  | 1:10:A:ARG:HD2  | 5        | 0.18          |
| (1,932)  | 1:10:A:ARG:HA  | 1:10:A:ARG:HD3  | 5        | 0.18          |
| (1,776)  | 1:52:A:ILE:HA  | 1:52:A:ILE:HD11 | 1        | 0.18          |
| (1,776)  | 1:52:A:ILE:HA  | 1:52:A:ILE:HD12 | 1        | 0.18          |
| (1,776)  | 1:52:A:ILE:HA  | 1:52:A:ILE:HD13 | 1        | 0.18          |
| (1,776)  | 1:52:A:ILE:HA  | 1:52:A:ILE:HD11 | 7        | 0.18          |
| (1,776)  | 1:52:A:ILE:HA  | 1:52:A:ILE:HD12 | 7        | 0.18          |
| (1,776)  | 1:52:A:ILE:HA  | 1:52:A:ILE:HD13 | 7        | 0.18          |
| (1,776)  | 1:52:A:ILE:HA  | 1:52:A:ILE:HD11 | 14       | 0.18          |
| (1,776)  | 1:52:A:ILE:HA  | 1:52:A:ILE:HD12 | 14       | 0.18          |
| (1,776)  | 1:52:A:ILE:HA  | 1:52:A:ILE:HD13 | 14       | 0.18          |
| (1,776)  | 1:52:A:ILE:HA  | 1:52:A:ILE:HD11 | 16       | 0.18          |
| (1,776)  | 1:52:A:ILE:HA  | 1:52:A:ILE:HD12 | 16       | 0.18          |
| (1,776)  | 1:52:A:ILE:HA  | 1:52:A:ILE:HD13 | 16       | 0.18          |
| (1,776)  | 1:52:A:ILE:HA  | 1:52:A:ILE:HD11 | 18       | 0.18          |
| (1,776)  | 1:52:A:ILE:HA  | 1:52:A:ILE:HD12 | 18       | 0.18          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD13 | 18       | 0.18          |
| (1,724) | 1:73:A:ILE:HA   | 1:73:A:ILE:HD11 | 10       | 0.18          |
| (1,724) | 1:73:A:ILE:HA   | 1:73:A:ILE:HD12 | 10       | 0.18          |
| (1,724) | 1:73:A:ILE:HA   | 1:73:A:ILE:HD13 | 10       | 0.18          |
| (1,717) | 1:53:A:VAL:HG11 | 1:60:A:TYR:HB3  | 1        | 0.18          |
| (1,717) | 1:53:A:VAL:HG12 | 1:60:A:TYR:HB3  | 1        | 0.18          |
| (1,717) | 1:53:A:VAL:HG13 | 1:60:A:TYR:HB3  | 1        | 0.18          |
| (1,717) | 1:53:A:VAL:HG21 | 1:60:A:TYR:HB3  | 1        | 0.18          |
| (1,717) | 1:53:A:VAL:HG22 | 1:60:A:TYR:HB3  | 1        | 0.18          |
| (1,717) | 1:53:A:VAL:HG23 | 1:60:A:TYR:HB3  | 1        | 0.18          |
| (1,717) | 1:53:A:VAL:HG11 | 1:60:A:TYR:HB3  | 8        | 0.18          |
| (1,717) | 1:53:A:VAL:HG12 | 1:60:A:TYR:HB3  | 8        | 0.18          |
| (1,717) | 1:53:A:VAL:HG13 | 1:60:A:TYR:HB3  | 8        | 0.18          |
| (1,717) | 1:53:A:VAL:HG21 | 1:60:A:TYR:HB3  | 8        | 0.18          |
| (1,717) | 1:53:A:VAL:HG22 | 1:60:A:TYR:HB3  | 8        | 0.18          |
| (1,717) | 1:53:A:VAL:HG23 | 1:60:A:TYR:HB3  | 8        | 0.18          |
| (1,717) | 1:53:A:VAL:HG11 | 1:60:A:TYR:HB3  | 13       | 0.18          |
| (1,717) | 1:53:A:VAL:HG12 | 1:60:A:TYR:HB3  | 13       | 0.18          |
| (1,717) | 1:53:A:VAL:HG13 | 1:60:A:TYR:HB3  | 13       | 0.18          |
| (1,717) | 1:53:A:VAL:HG21 | 1:60:A:TYR:HB3  | 13       | 0.18          |
| (1,717) | 1:53:A:VAL:HG22 | 1:60:A:TYR:HB3  | 13       | 0.18          |
| (1,717) | 1:53:A:VAL:HG23 | 1:60:A:TYR:HB3  | 13       | 0.18          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD21 | 11       | 0.18          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD22 | 11       | 0.18          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD23 | 11       | 0.18          |
| (1,689) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD11 | 18       | 0.18          |
| (1,689) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD12 | 18       | 0.18          |
| (1,689) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD13 | 18       | 0.18          |
| (1,649) | 1:52:A:ILE:HA   | 1:62:A:VAL:HG21 | 2        | 0.18          |
| (1,649) | 1:52:A:ILE:HA   | 1:62:A:VAL:HG22 | 2        | 0.18          |
| (1,649) | 1:52:A:ILE:HA   | 1:62:A:VAL:HG23 | 2        | 0.18          |
| (1,628) | 1:34:A:LYS:H    | 1:34:A:LYS:HG2  | 9        | 0.18          |
| (1,575) | 1:10:A:ARG:HA   | 1:10:A:ARG:HG3  | 14       | 0.18          |
| (1,561) | 1:39:A:ARG:HG2  | 1:43:A:TYR:HB2  | 9        | 0.18          |
| (1,561) | 1:39:A:ARG:HG2  | 1:43:A:TYR:HB3  | 9        | 0.18          |
| (1,561) | 1:39:A:ARG:HG3  | 1:43:A:TYR:HB2  | 9        | 0.18          |
| (1,561) | 1:39:A:ARG:HG3  | 1:43:A:TYR:HB3  | 9        | 0.18          |
| (1,556) | 1:29:A:GLU:HG2  | 1:60:A:TYR:HB2  | 11       | 0.18          |
| (1,556) | 1:29:A:GLU:HG3  | 1:60:A:TYR:HB2  | 11       | 0.18          |
| (1,556) | 1:29:A:GLU:HG2  | 1:60:A:TYR:HB2  | 18       | 0.18          |
| (1,556) | 1:29:A:GLU:HG3  | 1:60:A:TYR:HB2  | 18       | 0.18          |
| (1,485) | 1:43:A:TYR:HB2  | 1:47:A:ARG:HD2  | 10       | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,485)  | 1:43:A:TYR:HB2  | 1:47:A:ARG:HD3  | 10       | 0.18          |
| (1,485)  | 1:43:A:TYR:HB3  | 1:47:A:ARG:HD2  | 10       | 0.18          |
| (1,485)  | 1:43:A:TYR:HB3  | 1:47:A:ARG:HD3  | 10       | 0.18          |
| (1,409)  | 1:78:A:HIS:HB2  | 1:78:A:HIS:HD2  | 2        | 0.18          |
| (1,409)  | 1:78:A:HIS:HB2  | 1:78:A:HIS:HD2  | 4        | 0.18          |
| (1,409)  | 1:78:A:HIS:HB2  | 1:78:A:HIS:HD2  | 9        | 0.18          |
| (1,401)  | 1:32:A:TYR:HD1  | 1:55:A:ARG:HG2  | 12       | 0.18          |
| (1,401)  | 1:32:A:TYR:HD2  | 1:55:A:ARG:HG2  | 12       | 0.18          |
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG11 | 19       | 0.18          |
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG12 | 19       | 0.18          |
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG13 | 19       | 0.18          |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG11 | 19       | 0.18          |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG12 | 19       | 0.18          |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG13 | 19       | 0.18          |
| (1,316)  | 1:2:A:PHE:HD1   | 1:9:A:PRO:HD3   | 2        | 0.18          |
| (1,316)  | 1:2:A:PHE:HD2   | 1:9:A:PRO:HD3   | 2        | 0.18          |
| (1,283)  | 1:23:A:ILE:HG12 | 1:24:A:HIS:HE1  | 13       | 0.18          |
| (1,223)  | 1:7:A:GLU:H     | 1:7:A:GLU:HB3   | 13       | 0.18          |
| (1,165)  | 1:35:A:GLN:H    | 1:35:A:GLN:HB2  | 7        | 0.18          |
| (1,97)   | 1:36:A:GLN:H    | 1:36:A:GLN:HB3  | 5        | 0.18          |
| (1,97)   | 1:36:A:GLN:H    | 1:36:A:GLN:HB3  | 13       | 0.18          |
| (1,53)   | 1:37:A:LEU:H    | 1:37:A:LEU:HB3  | 3        | 0.18          |
| (1,53)   | 1:37:A:LEU:H    | 1:37:A:LEU:HB3  | 6        | 0.18          |
| (1,53)   | 1:37:A:LEU:H    | 1:37:A:LEU:HB3  | 8        | 0.18          |
| (1,53)   | 1:37:A:LEU:H    | 1:37:A:LEU:HB3  | 15       | 0.18          |
| (1,49)   | 1:55:A:ARG:H    | 1:59:A:PRO:HA   | 4        | 0.18          |
| (1,49)   | 1:55:A:ARG:H    | 1:59:A:PRO:HA   | 5        | 0.18          |
| (1,49)   | 1:55:A:ARG:H    | 1:59:A:PRO:HA   | 10       | 0.18          |
| (1,49)   | 1:55:A:ARG:H    | 1:59:A:PRO:HA   | 13       | 0.18          |
| (1,49)   | 1:55:A:ARG:H    | 1:59:A:PRO:HA   | 20       | 0.18          |
| (1,1253) | 1:32:A:TYR:HE1  | 1:62:A:VAL:HB   | 14       | 0.17          |
| (1,1253) | 1:32:A:TYR:HE2  | 1:62:A:VAL:HB   | 14       | 0.17          |
| (1,1253) | 1:32:A:TYR:HE1  | 1:62:A:VAL:HB   | 20       | 0.17          |
| (1,1253) | 1:32:A:TYR:HE2  | 1:62:A:VAL:HB   | 20       | 0.17          |
| (1,1229) | 1:55:A:ARG:HG3  | 1:32:A:TYR:H    | 3        | 0.17          |
| (1,1229) | 1:55:A:ARG:HG3  | 1:32:A:TYR:H    | 9        | 0.17          |
| (1,1228) | 1:9:A:PRO:HG2   | 1:54:A:TYR:HE1  | 20       | 0.17          |
| (1,1228) | 1:9:A:PRO:HG2   | 1:54:A:TYR:HE2  | 20       | 0.17          |
| (1,1228) | 1:9:A:PRO:HG3   | 1:54:A:TYR:HE1  | 20       | 0.17          |
| (1,1228) | 1:9:A:PRO:HG3   | 1:54:A:TYR:HE2  | 20       | 0.17          |
| (1,1170) | 1:48:A:ARG:H    | 1:48:A:ARG:HD3  | 12       | 0.17          |
| (1,1142) | 1:69:A:PHE:H    | 1:69:A:PHE:HB3  | 1        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1142) | 1:69:A:PHE:H    | 1:69:A:PHE:HB3  | 2        | 0.17          |
| (1,1142) | 1:69:A:PHE:H    | 1:69:A:PHE:HB3  | 5        | 0.17          |
| (1,1142) | 1:69:A:PHE:H    | 1:69:A:PHE:HB3  | 6        | 0.17          |
| (1,1142) | 1:69:A:PHE:H    | 1:69:A:PHE:HB3  | 18       | 0.17          |
| (1,1142) | 1:69:A:PHE:H    | 1:69:A:PHE:HB3  | 19       | 0.17          |
| (1,1114) | 1:36:A:GLN:H    | 1:36:A:GLN:HG3  | 8        | 0.17          |
| (1,1114) | 1:36:A:GLN:H    | 1:36:A:GLN:HG3  | 20       | 0.17          |
| (1,1056) | 1:31:A:VAL:HG11 | 1:55:A:ARG:HA   | 5        | 0.17          |
| (1,1056) | 1:31:A:VAL:HG12 | 1:55:A:ARG:HA   | 5        | 0.17          |
| (1,1056) | 1:31:A:VAL:HG13 | 1:55:A:ARG:HA   | 5        | 0.17          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB1  | 1        | 0.17          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB2  | 1        | 0.17          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB3  | 1        | 0.17          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB1  | 5        | 0.17          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB2  | 5        | 0.17          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB3  | 5        | 0.17          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB1  | 15       | 0.17          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB2  | 15       | 0.17          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB3  | 15       | 0.17          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB1  | 18       | 0.17          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB2  | 18       | 0.17          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB3  | 18       | 0.17          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD21 | 1        | 0.17          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD22 | 1        | 0.17          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD23 | 1        | 0.17          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD21 | 5        | 0.17          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD22 | 5        | 0.17          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD23 | 5        | 0.17          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD21 | 15       | 0.17          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD22 | 15       | 0.17          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD23 | 15       | 0.17          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD21 | 17       | 0.17          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD22 | 17       | 0.17          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD23 | 17       | 0.17          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD21 | 20       | 0.17          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD22 | 20       | 0.17          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD23 | 20       | 0.17          |
| (1,996)  | 1:10:A:ARG:HA   | 1:10:A:ARG:HG2  | 19       | 0.17          |
| (1,966)  | 1:33:A:CYS:HB2  | 1:35:A:GLN:HG2  | 2        | 0.17          |
| (1,966)  | 1:33:A:CYS:HB2  | 1:35:A:GLN:HG3  | 2        | 0.17          |
| (1,964)  | 1:53:A:VAL:HG21 | 1:62:A:VAL:HB   | 16       | 0.17          |
| (1,964)  | 1:53:A:VAL:HG22 | 1:62:A:VAL:HB   | 16       | 0.17          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,964) | 1:53:A:VAL:HG23 | 1:62:A:VAL:HB   | 16       | 0.17          |
| (1,958) | 1:29:A:GLU:HA   | 1:29:A:GLU:HG2  | 1        | 0.17          |
| (1,958) | 1:29:A:GLU:HA   | 1:29:A:GLU:HG3  | 1        | 0.17          |
| (1,958) | 1:29:A:GLU:HA   | 1:29:A:GLU:HG2  | 5        | 0.17          |
| (1,958) | 1:29:A:GLU:HA   | 1:29:A:GLU:HG3  | 5        | 0.17          |
| (1,958) | 1:29:A:GLU:HA   | 1:29:A:GLU:HG2  | 11       | 0.17          |
| (1,958) | 1:29:A:GLU:HA   | 1:29:A:GLU:HG3  | 11       | 0.17          |
| (1,958) | 1:29:A:GLU:HA   | 1:29:A:GLU:HG2  | 20       | 0.17          |
| (1,958) | 1:29:A:GLU:HA   | 1:29:A:GLU:HG3  | 20       | 0.17          |
| (1,924) | 1:9:A:PRO:HD2   | 1:15:A:LEU:HB3  | 6        | 0.17          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD11 | 3        | 0.17          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD12 | 3        | 0.17          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD13 | 3        | 0.17          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD11 | 5        | 0.17          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD12 | 5        | 0.17          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD13 | 5        | 0.17          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD11 | 9        | 0.17          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD12 | 9        | 0.17          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD13 | 9        | 0.17          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD11 | 13       | 0.17          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD12 | 13       | 0.17          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD13 | 13       | 0.17          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD11 | 17       | 0.17          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD12 | 17       | 0.17          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD13 | 17       | 0.17          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD11 | 19       | 0.17          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD12 | 19       | 0.17          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD13 | 19       | 0.17          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD11 | 20       | 0.17          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD12 | 20       | 0.17          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD13 | 20       | 0.17          |
| (1,724) | 1:73:A:ILE:HA   | 1:73:A:ILE:HD11 | 18       | 0.17          |
| (1,724) | 1:73:A:ILE:HA   | 1:73:A:ILE:HD12 | 18       | 0.17          |
| (1,724) | 1:73:A:ILE:HA   | 1:73:A:ILE:HD13 | 18       | 0.17          |
| (1,717) | 1:53:A:VAL:HG11 | 1:60:A:TYR:HB3  | 4        | 0.17          |
| (1,717) | 1:53:A:VAL:HG12 | 1:60:A:TYR:HB3  | 4        | 0.17          |
| (1,717) | 1:53:A:VAL:HG13 | 1:60:A:TYR:HB3  | 4        | 0.17          |
| (1,717) | 1:53:A:VAL:HG21 | 1:60:A:TYR:HB3  | 4        | 0.17          |
| (1,717) | 1:53:A:VAL:HG22 | 1:60:A:TYR:HB3  | 4        | 0.17          |
| (1,717) | 1:53:A:VAL:HG23 | 1:60:A:TYR:HB3  | 4        | 0.17          |
| (1,717) | 1:53:A:VAL:HG11 | 1:60:A:TYR:HB3  | 5        | 0.17          |
| (1,717) | 1:53:A:VAL:HG12 | 1:60:A:TYR:HB3  | 5        | 0.17          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,717) | 1:53:A:VAL:HG13 | 1:60:A:TYR:HB3  | 5        | 0.17          |
| (1,717) | 1:53:A:VAL:HG21 | 1:60:A:TYR:HB3  | 5        | 0.17          |
| (1,717) | 1:53:A:VAL:HG22 | 1:60:A:TYR:HB3  | 5        | 0.17          |
| (1,717) | 1:53:A:VAL:HG23 | 1:60:A:TYR:HB3  | 5        | 0.17          |
| (1,689) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD11 | 3        | 0.17          |
| (1,689) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD12 | 3        | 0.17          |
| (1,689) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD13 | 3        | 0.17          |
| (1,649) | 1:52:A:ILE:HA   | 1:62:A:VAL:HG21 | 1        | 0.17          |
| (1,649) | 1:52:A:ILE:HA   | 1:62:A:VAL:HG22 | 1        | 0.17          |
| (1,649) | 1:52:A:ILE:HA   | 1:62:A:VAL:HG23 | 1        | 0.17          |
| (1,628) | 1:34:A:LYS:H    | 1:34:A:LYS:HG2  | 20       | 0.17          |
| (1,625) | 1:8:A:ARG:HG2   | 1:59:A:PRO:HG2  | 13       | 0.17          |
| (1,625) | 1:8:A:ARG:HG3   | 1:59:A:PRO:HG2  | 13       | 0.17          |
| (1,625) | 1:8:A:ARG:HG2   | 1:59:A:PRO:HG2  | 14       | 0.17          |
| (1,625) | 1:8:A:ARG:HG3   | 1:59:A:PRO:HG2  | 14       | 0.17          |
| (1,599) | 1:37:A:LEU:HA   | 1:38:A:LEU:HB3  | 5        | 0.17          |
| (1,595) | 1:16:A:CYS:HA   | 1:19:A:LEU:HB3  | 14       | 0.17          |
| (1,575) | 1:10:A:ARG:HA   | 1:10:A:ARG:HG3  | 7        | 0.17          |
| (1,556) | 1:29:A:GLU:HG2  | 1:60:A:TYR:HB2  | 13       | 0.17          |
| (1,556) | 1:29:A:GLU:HG3  | 1:60:A:TYR:HB2  | 13       | 0.17          |
| (1,547) | 1:8:A:ARG:HB2   | 1:59:A:PRO:HG3  | 9        | 0.17          |
| (1,547) | 1:8:A:ARG:HB3   | 1:59:A:PRO:HG3  | 9        | 0.17          |
| (1,467) | 1:54:A:TYR:HE1  | 1:58:A:ASN:HA   | 10       | 0.17          |
| (1,467) | 1:54:A:TYR:HE2  | 1:58:A:ASN:HA   | 10       | 0.17          |
| (1,467) | 1:54:A:TYR:HE1  | 1:58:A:ASN:HA   | 13       | 0.17          |
| (1,467) | 1:54:A:TYR:HE2  | 1:58:A:ASN:HA   | 13       | 0.17          |
| (1,465) | 1:32:A:TYR:HE1  | 1:55:A:ARG:HG2  | 15       | 0.17          |
| (1,465) | 1:32:A:TYR:HE2  | 1:55:A:ARG:HG2  | 15       | 0.17          |
| (1,430) | 1:3:A:GLN:HA    | 1:3:A:GLN:HE22  | 4        | 0.17          |
| (1,430) | 1:3:A:GLN:HA    | 1:3:A:GLN:HE22  | 11       | 0.17          |
| (1,409) | 1:78:A:HIS:HB2  | 1:78:A:HIS:HD2  | 12       | 0.17          |
| (1,401) | 1:32:A:TYR:HD1  | 1:55:A:ARG:HG2  | 14       | 0.17          |
| (1,401) | 1:32:A:TYR:HD2  | 1:55:A:ARG:HG2  | 14       | 0.17          |
| (1,334) | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG11 | 1        | 0.17          |
| (1,334) | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG12 | 1        | 0.17          |
| (1,334) | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG13 | 1        | 0.17          |
| (1,334) | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG11 | 1        | 0.17          |
| (1,334) | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG12 | 1        | 0.17          |
| (1,334) | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG13 | 1        | 0.17          |
| (1,334) | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG11 | 2        | 0.17          |
| (1,334) | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG12 | 2        | 0.17          |
| (1,334) | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG13 | 2        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG11 | 2        | 0.17          |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG12 | 2        | 0.17          |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG13 | 2        | 0.17          |
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG11 | 9        | 0.17          |
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG12 | 9        | 0.17          |
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG13 | 9        | 0.17          |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG11 | 9        | 0.17          |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG12 | 9        | 0.17          |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG13 | 9        | 0.17          |
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG11 | 13       | 0.17          |
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG12 | 13       | 0.17          |
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG13 | 13       | 0.17          |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG11 | 13       | 0.17          |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG12 | 13       | 0.17          |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG13 | 13       | 0.17          |
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG11 | 15       | 0.17          |
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG12 | 15       | 0.17          |
| (1,334)  | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG13 | 15       | 0.17          |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG11 | 15       | 0.17          |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG12 | 15       | 0.17          |
| (1,334)  | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG13 | 15       | 0.17          |
| (1,283)  | 1:23:A:ILE:HG12 | 1:24:A:HIS:HE1  | 2        | 0.17          |
| (1,241)  | 1:34:A:LYS:H    | 1:34:A:LYS:HG3  | 13       | 0.17          |
| (1,223)  | 1:7:A:GLU:H     | 1:7:A:GLU:HB3   | 3        | 0.17          |
| (1,165)  | 1:35:A:GLN:H    | 1:35:A:GLN:HB2  | 1        | 0.17          |
| (1,128)  | 1:5:A:PRO:HD3   | 1:6:A:GLN:H     | 10       | 0.17          |
| (1,82)   | 1:54:A:TYR:H    | 1:59:A:PRO:HA   | 12       | 0.17          |
| (1,53)   | 1:37:A:LEU:H    | 1:37:A:LEU:HB3  | 1        | 0.17          |
| (1,53)   | 1:37:A:LEU:H    | 1:37:A:LEU:HB3  | 12       | 0.17          |
| (1,53)   | 1:37:A:LEU:H    | 1:37:A:LEU:HB3  | 17       | 0.17          |
| (1,53)   | 1:37:A:LEU:H    | 1:37:A:LEU:HB3  | 20       | 0.17          |
| (1,49)   | 1:55:A:ARG:H    | 1:59:A:PRO:HA   | 1        | 0.17          |
| (1,49)   | 1:55:A:ARG:H    | 1:59:A:PRO:HA   | 2        | 0.17          |
| (1,49)   | 1:55:A:ARG:H    | 1:59:A:PRO:HA   | 3        | 0.17          |
| (1,49)   | 1:55:A:ARG:H    | 1:59:A:PRO:HA   | 6        | 0.17          |
| (1,49)   | 1:55:A:ARG:H    | 1:59:A:PRO:HA   | 7        | 0.17          |
| (1,49)   | 1:55:A:ARG:H    | 1:59:A:PRO:HA   | 14       | 0.17          |
| (1,49)   | 1:55:A:ARG:H    | 1:59:A:PRO:HA   | 16       | 0.17          |
| (1,49)   | 1:55:A:ARG:H    | 1:59:A:PRO:HA   | 18       | 0.17          |
| (1,1253) | 1:32:A:TYR:HE1  | 1:62:A:VAL:HB   | 9        | 0.16          |
| (1,1253) | 1:32:A:TYR:HE2  | 1:62:A:VAL:HB   | 9        | 0.16          |
| (1,1253) | 1:32:A:TYR:HE1  | 1:62:A:VAL:HB   | 11       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1253) | 1:32:A:TYR:HE2  | 1:62:A:VAL:HB   | 11       | 0.16          |
| (1,1253) | 1:32:A:TYR:HE1  | 1:62:A:VAL:HB   | 19       | 0.16          |
| (1,1253) | 1:32:A:TYR:HE2  | 1:62:A:VAL:HB   | 19       | 0.16          |
| (1,1234) | 1:10:A:ARG:HA   | 1:52:A:ILE:HD11 | 3        | 0.16          |
| (1,1234) | 1:10:A:ARG:HA   | 1:52:A:ILE:HD12 | 3        | 0.16          |
| (1,1234) | 1:10:A:ARG:HA   | 1:52:A:ILE:HD13 | 3        | 0.16          |
| (1,1234) | 1:10:A:ARG:HA   | 1:52:A:ILE:HD11 | 4        | 0.16          |
| (1,1234) | 1:10:A:ARG:HA   | 1:52:A:ILE:HD12 | 4        | 0.16          |
| (1,1234) | 1:10:A:ARG:HA   | 1:52:A:ILE:HD13 | 4        | 0.16          |
| (1,1228) | 1:9:A:PRO:HG2   | 1:54:A:TYR:HE1  | 18       | 0.16          |
| (1,1228) | 1:9:A:PRO:HG2   | 1:54:A:TYR:HE2  | 18       | 0.16          |
| (1,1228) | 1:9:A:PRO:HG3   | 1:54:A:TYR:HE1  | 18       | 0.16          |
| (1,1228) | 1:9:A:PRO:HG3   | 1:54:A:TYR:HE2  | 18       | 0.16          |
| (1,1225) | 1:2:A:PHE:HE1   | 1:54:A:TYR:HE1  | 2        | 0.16          |
| (1,1225) | 1:2:A:PHE:HE1   | 1:54:A:TYR:HE2  | 2        | 0.16          |
| (1,1225) | 1:2:A:PHE:HE2   | 1:54:A:TYR:HE1  | 2        | 0.16          |
| (1,1225) | 1:2:A:PHE:HE2   | 1:54:A:TYR:HE2  | 2        | 0.16          |
| (1,1215) | 1:3:A:GLN:HE22  | 1:4:A:ASP:HA    | 5        | 0.16          |
| (1,1177) | 1:19:A:LEU:H    | 1:19:A:LEU:HG   | 1        | 0.16          |
| (1,1170) | 1:48:A:ARG:H    | 1:48:A:ARG:HD3  | 13       | 0.16          |
| (1,1165) | 1:6:A:GLN:H     | 1:6:A:GLN:HB2   | 7        | 0.16          |
| (1,1145) | 1:73:A:ILE:H    | 1:73:A:ILE:HB   | 18       | 0.16          |
| (1,1142) | 1:69:A:PHE:H    | 1:69:A:PHE:HB3  | 11       | 0.16          |
| (1,1118) | 1:7:A:GLU:HA    | 1:8:A:ARG:H     | 20       | 0.16          |
| (1,1072) | 1:29:A:GLU:HB2  | 1:37:A:LEU:H    | 7        | 0.16          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB1  | 2        | 0.16          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB2  | 2        | 0.16          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB3  | 2        | 0.16          |
| (1,1035) | 1:17:A:THR:HG21 | 1:18:A:GLU:HG3  | 3        | 0.16          |
| (1,1035) | 1:17:A:THR:HG22 | 1:18:A:GLU:HG3  | 3        | 0.16          |
| (1,1035) | 1:17:A:THR:HG23 | 1:18:A:GLU:HG3  | 3        | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD21 | 2        | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD22 | 2        | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD23 | 2        | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD21 | 3        | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD22 | 3        | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD23 | 3        | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD21 | 4        | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD22 | 4        | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD23 | 4        | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD21 | 6        | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD22 | 6        | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD23 | 6        | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD21 | 9        | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD22 | 9        | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD23 | 9        | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD21 | 10       | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD22 | 10       | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD23 | 10       | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD21 | 12       | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD22 | 12       | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD23 | 12       | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD21 | 13       | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD22 | 13       | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD23 | 13       | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD21 | 14       | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD22 | 14       | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD23 | 14       | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD21 | 16       | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD22 | 16       | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD23 | 16       | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD21 | 18       | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD22 | 18       | 0.16          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD23 | 18       | 0.16          |
| (1,958)  | 1:29:A:GLU:HA   | 1:29:A:GLU:HG2  | 10       | 0.16          |
| (1,958)  | 1:29:A:GLU:HA   | 1:29:A:GLU:HG3  | 10       | 0.16          |
| (1,958)  | 1:29:A:GLU:HA   | 1:29:A:GLU:HG2  | 13       | 0.16          |
| (1,958)  | 1:29:A:GLU:HA   | 1:29:A:GLU:HG3  | 13       | 0.16          |
| (1,958)  | 1:29:A:GLU:HA   | 1:29:A:GLU:HG2  | 17       | 0.16          |
| (1,958)  | 1:29:A:GLU:HA   | 1:29:A:GLU:HG3  | 17       | 0.16          |
| (1,958)  | 1:29:A:GLU:HA   | 1:29:A:GLU:HG2  | 18       | 0.16          |
| (1,958)  | 1:29:A:GLU:HA   | 1:29:A:GLU:HG3  | 18       | 0.16          |
| (1,958)  | 1:29:A:GLU:HA   | 1:29:A:GLU:HG2  | 19       | 0.16          |
| (1,958)  | 1:29:A:GLU:HA   | 1:29:A:GLU:HG3  | 19       | 0.16          |
| (1,956)  | 1:18:A:GLU:H    | 1:18:A:GLU:HG2  | 14       | 0.16          |
| (1,924)  | 1:9:A:PRO:HD2   | 1:15:A:LEU:HB3  | 2        | 0.16          |
| (1,924)  | 1:9:A:PRO:HD2   | 1:15:A:LEU:HB3  | 10       | 0.16          |
| (1,916)  | 1:8:A:ARG:HA    | 1:8:A:ARG:HG2   | 2        | 0.16          |
| (1,916)  | 1:8:A:ARG:HA    | 1:8:A:ARG:HG3   | 2        | 0.16          |
| (1,888)  | 1:44:A:ASP:HA   | 1:47:A:ARG:H    | 1        | 0.16          |
| (1,888)  | 1:44:A:ASP:HA   | 1:47:A:ARG:H    | 4        | 0.16          |
| (1,867)  | 1:15:A:LEU:HD11 | 1:18:A:GLU:HA   | 14       | 0.16          |
| (1,867)  | 1:15:A:LEU:HD12 | 1:18:A:GLU:HA   | 14       | 0.16          |
| (1,867)  | 1:15:A:LEU:HD13 | 1:18:A:GLU:HA   | 14       | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,866) | 1:65:A:LYS:HA   | 1:65:A:LYS:HG3  | 10       | 0.16          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD11 | 2        | 0.16          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD12 | 2        | 0.16          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD13 | 2        | 0.16          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD11 | 10       | 0.16          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD12 | 10       | 0.16          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD13 | 10       | 0.16          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD11 | 12       | 0.16          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD12 | 12       | 0.16          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD13 | 12       | 0.16          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD11 | 15       | 0.16          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD12 | 15       | 0.16          |
| (1,776) | 1:52:A:ILE:HA   | 1:52:A:ILE:HD13 | 15       | 0.16          |
| (1,724) | 1:73:A:ILE:HA   | 1:73:A:ILE:HD11 | 9        | 0.16          |
| (1,724) | 1:73:A:ILE:HA   | 1:73:A:ILE:HD12 | 9        | 0.16          |
| (1,724) | 1:73:A:ILE:HA   | 1:73:A:ILE:HD13 | 9        | 0.16          |
| (1,717) | 1:53:A:VAL:HG11 | 1:60:A:TYR:HB3  | 3        | 0.16          |
| (1,717) | 1:53:A:VAL:HG12 | 1:60:A:TYR:HB3  | 3        | 0.16          |
| (1,717) | 1:53:A:VAL:HG13 | 1:60:A:TYR:HB3  | 3        | 0.16          |
| (1,717) | 1:53:A:VAL:HG21 | 1:60:A:TYR:HB3  | 3        | 0.16          |
| (1,717) | 1:53:A:VAL:HG22 | 1:60:A:TYR:HB3  | 3        | 0.16          |
| (1,717) | 1:53:A:VAL:HG23 | 1:60:A:TYR:HB3  | 3        | 0.16          |
| (1,717) | 1:53:A:VAL:HG11 | 1:60:A:TYR:HB3  | 6        | 0.16          |
| (1,717) | 1:53:A:VAL:HG12 | 1:60:A:TYR:HB3  | 6        | 0.16          |
| (1,717) | 1:53:A:VAL:HG13 | 1:60:A:TYR:HB3  | 6        | 0.16          |
| (1,717) | 1:53:A:VAL:HG21 | 1:60:A:TYR:HB3  | 6        | 0.16          |
| (1,717) | 1:53:A:VAL:HG22 | 1:60:A:TYR:HB3  | 6        | 0.16          |
| (1,717) | 1:53:A:VAL:HG23 | 1:60:A:TYR:HB3  | 6        | 0.16          |
| (1,717) | 1:53:A:VAL:HG11 | 1:60:A:TYR:HB3  | 10       | 0.16          |
| (1,717) | 1:53:A:VAL:HG12 | 1:60:A:TYR:HB3  | 10       | 0.16          |
| (1,717) | 1:53:A:VAL:HG13 | 1:60:A:TYR:HB3  | 10       | 0.16          |
| (1,717) | 1:53:A:VAL:HG21 | 1:60:A:TYR:HB3  | 10       | 0.16          |
| (1,717) | 1:53:A:VAL:HG22 | 1:60:A:TYR:HB3  | 10       | 0.16          |
| (1,717) | 1:53:A:VAL:HG23 | 1:60:A:TYR:HB3  | 10       | 0.16          |
| (1,717) | 1:53:A:VAL:HG11 | 1:60:A:TYR:HB3  | 12       | 0.16          |
| (1,717) | 1:53:A:VAL:HG12 | 1:60:A:TYR:HB3  | 12       | 0.16          |
| (1,717) | 1:53:A:VAL:HG13 | 1:60:A:TYR:HB3  | 12       | 0.16          |
| (1,717) | 1:53:A:VAL:HG21 | 1:60:A:TYR:HB3  | 12       | 0.16          |
| (1,717) | 1:53:A:VAL:HG22 | 1:60:A:TYR:HB3  | 12       | 0.16          |
| (1,717) | 1:53:A:VAL:HG23 | 1:60:A:TYR:HB3  | 12       | 0.16          |
| (1,717) | 1:53:A:VAL:HG11 | 1:60:A:TYR:HB3  | 17       | 0.16          |
| (1,717) | 1:53:A:VAL:HG12 | 1:60:A:TYR:HB3  | 17       | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,717) | 1:53:A:VAL:HG13 | 1:60:A:TYR:HB3  | 17       | 0.16          |
| (1,717) | 1:53:A:VAL:HG21 | 1:60:A:TYR:HB3  | 17       | 0.16          |
| (1,717) | 1:53:A:VAL:HG22 | 1:60:A:TYR:HB3  | 17       | 0.16          |
| (1,717) | 1:53:A:VAL:HG23 | 1:60:A:TYR:HB3  | 17       | 0.16          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD21 | 6        | 0.16          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD22 | 6        | 0.16          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD23 | 6        | 0.16          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD21 | 7        | 0.16          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD22 | 7        | 0.16          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD23 | 7        | 0.16          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD21 | 8        | 0.16          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD22 | 8        | 0.16          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD23 | 8        | 0.16          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD21 | 9        | 0.16          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD22 | 9        | 0.16          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD23 | 9        | 0.16          |
| (1,649) | 1:52:A:ILE:HA   | 1:62:A:VAL:HG21 | 9        | 0.16          |
| (1,649) | 1:52:A:ILE:HA   | 1:62:A:VAL:HG22 | 9        | 0.16          |
| (1,649) | 1:52:A:ILE:HA   | 1:62:A:VAL:HG23 | 9        | 0.16          |
| (1,628) | 1:34:A:LYS:H    | 1:34:A:LYS:HG2  | 8        | 0.16          |
| (1,628) | 1:34:A:LYS:H    | 1:34:A:LYS:HG2  | 14       | 0.16          |
| (1,625) | 1:8:A:ARG:HG2   | 1:59:A:PRO:HG2  | 6        | 0.16          |
| (1,625) | 1:8:A:ARG:HG3   | 1:59:A:PRO:HG2  | 6        | 0.16          |
| (1,625) | 1:8:A:ARG:HG2   | 1:59:A:PRO:HG2  | 12       | 0.16          |
| (1,625) | 1:8:A:ARG:HG3   | 1:59:A:PRO:HG2  | 12       | 0.16          |
| (1,625) | 1:8:A:ARG:HG2   | 1:59:A:PRO:HG2  | 16       | 0.16          |
| (1,625) | 1:8:A:ARG:HG3   | 1:59:A:PRO:HG2  | 16       | 0.16          |
| (1,595) | 1:16:A:CYS:HA   | 1:19:A:LEU:HB3  | 17       | 0.16          |
| (1,575) | 1:10:A:ARG:HA   | 1:10:A:ARG:HG3  | 15       | 0.16          |
| (1,575) | 1:10:A:ARG:HA   | 1:10:A:ARG:HG3  | 17       | 0.16          |
| (1,574) | 1:11:A:LYS:HA   | 1:11:A:LYS:HD2  | 20       | 0.16          |
| (1,574) | 1:11:A:LYS:HA   | 1:11:A:LYS:HD3  | 20       | 0.16          |
| (1,556) | 1:29:A:GLU:HG2  | 1:60:A:TYR:HB2  | 17       | 0.16          |
| (1,556) | 1:29:A:GLU:HG3  | 1:60:A:TYR:HB2  | 17       | 0.16          |
| (1,547) | 1:8:A:ARG:HB2   | 1:59:A:PRO:HG3  | 16       | 0.16          |
| (1,547) | 1:8:A:ARG:HB3   | 1:59:A:PRO:HG3  | 16       | 0.16          |
| (1,540) | 1:11:A:LYS:HB2  | 1:11:A:LYS:HD2  | 15       | 0.16          |
| (1,540) | 1:11:A:LYS:HB2  | 1:11:A:LYS:HD3  | 15       | 0.16          |
| (1,538) | 1:18:A:GLU:HB3  | 1:19:A:LEU:H    | 6        | 0.16          |
| (1,538) | 1:18:A:GLU:HB3  | 1:19:A:LEU:H    | 16       | 0.16          |
| (1,486) | 1:43:A:TYR:HB2  | 1:47:A:ARG:HB3  | 7        | 0.16          |
| (1,486) | 1:43:A:TYR:HB3  | 1:47:A:ARG:HB3  | 7        | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,478) | 1:8:A:ARG:HG2   | 1:59:A:PRO:HD2  | 14       | 0.16          |
| (1,478) | 1:8:A:ARG:HG3   | 1:59:A:PRO:HD2  | 14       | 0.16          |
| (1,455) | 1:54:A:TYR:HD1  | 1:59:A:PRO:HB2  | 7        | 0.16          |
| (1,455) | 1:54:A:TYR:HD2  | 1:59:A:PRO:HB2  | 7        | 0.16          |
| (1,455) | 1:54:A:TYR:HD1  | 1:59:A:PRO:HB2  | 20       | 0.16          |
| (1,455) | 1:54:A:TYR:HD2  | 1:59:A:PRO:HB2  | 20       | 0.16          |
| (1,418) | 1:29:A:GLU:HG2  | 1:60:A:TYR:HD1  | 7        | 0.16          |
| (1,418) | 1:29:A:GLU:HG2  | 1:60:A:TYR:HD2  | 7        | 0.16          |
| (1,418) | 1:29:A:GLU:HG3  | 1:60:A:TYR:HD1  | 7        | 0.16          |
| (1,418) | 1:29:A:GLU:HG3  | 1:60:A:TYR:HD2  | 7        | 0.16          |
| (1,409) | 1:78:A:HIS:HB2  | 1:78:A:HIS:HD2  | 20       | 0.16          |
| (1,401) | 1:32:A:TYR:HD1  | 1:55:A:ARG:HG2  | 18       | 0.16          |
| (1,401) | 1:32:A:TYR:HD2  | 1:55:A:ARG:HG2  | 18       | 0.16          |
| (1,382) | 1:78:A:HIS:HB3  | 1:79:A:TYR:HD1  | 11       | 0.16          |
| (1,382) | 1:78:A:HIS:HB3  | 1:79:A:TYR:HD2  | 11       | 0.16          |
| (1,334) | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG11 | 8        | 0.16          |
| (1,334) | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG12 | 8        | 0.16          |
| (1,334) | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG13 | 8        | 0.16          |
| (1,334) | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG11 | 8        | 0.16          |
| (1,334) | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG12 | 8        | 0.16          |
| (1,334) | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG13 | 8        | 0.16          |
| (1,334) | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG11 | 10       | 0.16          |
| (1,334) | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG12 | 10       | 0.16          |
| (1,334) | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG13 | 10       | 0.16          |
| (1,334) | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG11 | 10       | 0.16          |
| (1,334) | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG12 | 10       | 0.16          |
| (1,334) | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG13 | 10       | 0.16          |
| (1,321) | 1:2:A:PHE:HD1   | 1:19:A:LEU:HG   | 17       | 0.16          |
| (1,321) | 1:2:A:PHE:HD2   | 1:19:A:LEU:HG   | 17       | 0.16          |
| (1,316) | 1:2:A:PHE:HD1   | 1:9:A:PRO:HD3   | 8        | 0.16          |
| (1,316) | 1:2:A:PHE:HD2   | 1:9:A:PRO:HD3   | 8        | 0.16          |
| (1,310) | 1:2:A:PHE:HD1   | 1:8:A:ARG:H     | 20       | 0.16          |
| (1,310) | 1:2:A:PHE:HD2   | 1:8:A:ARG:H     | 20       | 0.16          |
| (1,306) | 1:45:A:PHE:HZ   | 1:52:A:ILE:HD11 | 16       | 0.16          |
| (1,306) | 1:45:A:PHE:HZ   | 1:52:A:ILE:HD12 | 16       | 0.16          |
| (1,306) | 1:45:A:PHE:HZ   | 1:52:A:ILE:HD13 | 16       | 0.16          |
| (1,287) | 1:7:A:GLU:HB2   | 1:8:A:ARG:H     | 12       | 0.16          |
| (1,283) | 1:23:A:ILE:HG12 | 1:24:A:HIS:HE1  | 4        | 0.16          |
| (1,283) | 1:23:A:ILE:HG12 | 1:24:A:HIS:HE1  | 11       | 0.16          |
| (1,241) | 1:34:A:LYS:H    | 1:34:A:LYS:HG3  | 12       | 0.16          |
| (1,116) | 1:44:A:ASP:H    | 1:44:A:ASP:HB3  | 4        | 0.16          |
| (1,116) | 1:44:A:ASP:H    | 1:44:A:ASP:HB3  | 10       | 0.16          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,116)  | 1:44:A:ASP:H   | 1:44:A:ASP:HB3  | 15       | 0.16          |
| (1,116)  | 1:44:A:ASP:H   | 1:44:A:ASP:HB3  | 20       | 0.16          |
| (1,96)   | 1:35:A:GLN:HB2 | 1:36:A:GLN:H    | 15       | 0.16          |
| (1,96)   | 1:35:A:GLN:HB2 | 1:36:A:GLN:H    | 17       | 0.16          |
| (1,82)   | 1:54:A:TYR:H   | 1:59:A:PRO:HA   | 2        | 0.16          |
| (1,82)   | 1:54:A:TYR:H   | 1:59:A:PRO:HA   | 9        | 0.16          |
| (1,82)   | 1:54:A:TYR:H   | 1:59:A:PRO:HA   | 10       | 0.16          |
| (1,82)   | 1:54:A:TYR:H   | 1:59:A:PRO:HA   | 15       | 0.16          |
| (1,82)   | 1:54:A:TYR:H   | 1:59:A:PRO:HA   | 16       | 0.16          |
| (1,82)   | 1:54:A:TYR:H   | 1:59:A:PRO:HA   | 17       | 0.16          |
| (1,53)   | 1:37:A:LEU:H   | 1:37:A:LEU:HB3  | 10       | 0.16          |
| (1,53)   | 1:37:A:LEU:H   | 1:37:A:LEU:HB3  | 13       | 0.16          |
| (1,45)   | 1:36:A:GLN:HG3 | 1:37:A:LEU:H    | 12       | 0.16          |
| (1,1253) | 1:32:A:TYR:HE1 | 1:62:A:VAL:HB   | 1        | 0.15          |
| (1,1253) | 1:32:A:TYR:HE2 | 1:62:A:VAL:HB   | 1        | 0.15          |
| (1,1253) | 1:32:A:TYR:HE1 | 1:62:A:VAL:HB   | 4        | 0.15          |
| (1,1253) | 1:32:A:TYR:HE2 | 1:62:A:VAL:HB   | 4        | 0.15          |
| (1,1253) | 1:32:A:TYR:HE1 | 1:62:A:VAL:HB   | 16       | 0.15          |
| (1,1253) | 1:32:A:TYR:HE2 | 1:62:A:VAL:HB   | 16       | 0.15          |
| (1,1242) | 1:29:A:GLU:HB2 | 1:60:A:TYR:HB2  | 4        | 0.15          |
| (1,1234) | 1:10:A:ARG:HA  | 1:52:A:ILE:HD11 | 9        | 0.15          |
| (1,1234) | 1:10:A:ARG:HA  | 1:52:A:ILE:HD12 | 9        | 0.15          |
| (1,1234) | 1:10:A:ARG:HA  | 1:52:A:ILE:HD13 | 9        | 0.15          |
| (1,1234) | 1:10:A:ARG:HA  | 1:52:A:ILE:HD11 | 15       | 0.15          |
| (1,1234) | 1:10:A:ARG:HA  | 1:52:A:ILE:HD12 | 15       | 0.15          |
| (1,1234) | 1:10:A:ARG:HA  | 1:52:A:ILE:HD13 | 15       | 0.15          |
| (1,1234) | 1:10:A:ARG:HA  | 1:52:A:ILE:HD11 | 17       | 0.15          |
| (1,1234) | 1:10:A:ARG:HA  | 1:52:A:ILE:HD12 | 17       | 0.15          |
| (1,1234) | 1:10:A:ARG:HA  | 1:52:A:ILE:HD13 | 17       | 0.15          |
| (1,1234) | 1:10:A:ARG:HA  | 1:52:A:ILE:HD11 | 19       | 0.15          |
| (1,1234) | 1:10:A:ARG:HA  | 1:52:A:ILE:HD12 | 19       | 0.15          |
| (1,1234) | 1:10:A:ARG:HA  | 1:52:A:ILE:HD13 | 19       | 0.15          |
| (1,1229) | 1:55:A:ARG:HG3 | 1:32:A:TYR:H    | 6        | 0.15          |
| (1,1225) | 1:2:A:PHE:HE1  | 1:54:A:TYR:HE1  | 8        | 0.15          |
| (1,1225) | 1:2:A:PHE:HE1  | 1:54:A:TYR:HE2  | 8        | 0.15          |
| (1,1225) | 1:2:A:PHE:HE2  | 1:54:A:TYR:HE1  | 8        | 0.15          |
| (1,1225) | 1:2:A:PHE:HE2  | 1:54:A:TYR:HE2  | 8        | 0.15          |
| (1,1225) | 1:2:A:PHE:HE1  | 1:54:A:TYR:HE1  | 11       | 0.15          |
| (1,1225) | 1:2:A:PHE:HE1  | 1:54:A:TYR:HE2  | 11       | 0.15          |
| (1,1225) | 1:2:A:PHE:HE2  | 1:54:A:TYR:HE1  | 11       | 0.15          |
| (1,1225) | 1:2:A:PHE:HE2  | 1:54:A:TYR:HE2  | 11       | 0.15          |
| (1,1177) | 1:19:A:LEU:H   | 1:19:A:LEU:HG   | 13       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1164) | 1:6:A:GLN:H     | 1:6:A:GLN:HG2   | 10       | 0.15          |
| (1,1164) | 1:6:A:GLN:H     | 1:6:A:GLN:HG3   | 10       | 0.15          |
| (1,1140) | 1:29:A:GLU:H    | 1:29:A:GLU:HB2  | 6        | 0.15          |
| (1,1118) | 1:7:A:GLU:HA    | 1:8:A:ARG:H     | 1        | 0.15          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB1  | 7        | 0.15          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB2  | 7        | 0.15          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB3  | 7        | 0.15          |
| (1,1035) | 1:17:A:THR:HG21 | 1:18:A:GLU:HG3  | 18       | 0.15          |
| (1,1035) | 1:17:A:THR:HG22 | 1:18:A:GLU:HG3  | 18       | 0.15          |
| (1,1035) | 1:17:A:THR:HG23 | 1:18:A:GLU:HG3  | 18       | 0.15          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG11 | 7        | 0.15          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG12 | 7        | 0.15          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG13 | 7        | 0.15          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD21 | 7        | 0.15          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD22 | 7        | 0.15          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD23 | 7        | 0.15          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD21 | 11       | 0.15          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD22 | 11       | 0.15          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD23 | 11       | 0.15          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD21 | 19       | 0.15          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD22 | 19       | 0.15          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD23 | 19       | 0.15          |
| (1,996)  | 1:10:A:ARG:HA   | 1:10:A:ARG:HG2  | 18       | 0.15          |
| (1,984)  | 1:26:A:ILE:HG13 | 1:28:A:LEU:HA   | 16       | 0.15          |
| (1,958)  | 1:29:A:GLU:HA   | 1:29:A:GLU:HG2  | 4        | 0.15          |
| (1,958)  | 1:29:A:GLU:HA   | 1:29:A:GLU:HG3  | 4        | 0.15          |
| (1,916)  | 1:8:A:ARG:HA    | 1:8:A:ARG:HG2   | 14       | 0.15          |
| (1,916)  | 1:8:A:ARG:HA    | 1:8:A:ARG:HG3   | 14       | 0.15          |
| (1,888)  | 1:44:A:ASP:HA   | 1:47:A:ARG:H    | 3        | 0.15          |
| (1,888)  | 1:44:A:ASP:HA   | 1:47:A:ARG:H    | 9        | 0.15          |
| (1,867)  | 1:15:A:LEU:HD11 | 1:18:A:GLU:HA   | 20       | 0.15          |
| (1,867)  | 1:15:A:LEU:HD12 | 1:18:A:GLU:HA   | 20       | 0.15          |
| (1,867)  | 1:15:A:LEU:HD13 | 1:18:A:GLU:HA   | 20       | 0.15          |
| (1,850)  | 1:23:A:ILE:HA   | 1:23:A:ILE:HG13 | 18       | 0.15          |
| (1,776)  | 1:52:A:ILE:HA   | 1:52:A:ILE:HD11 | 6        | 0.15          |
| (1,776)  | 1:52:A:ILE:HA   | 1:52:A:ILE:HD12 | 6        | 0.15          |
| (1,776)  | 1:52:A:ILE:HA   | 1:52:A:ILE:HD13 | 6        | 0.15          |
| (1,776)  | 1:52:A:ILE:HA   | 1:52:A:ILE:HD11 | 11       | 0.15          |
| (1,776)  | 1:52:A:ILE:HA   | 1:52:A:ILE:HD12 | 11       | 0.15          |
| (1,776)  | 1:52:A:ILE:HA   | 1:52:A:ILE:HD13 | 11       | 0.15          |
| (1,717)  | 1:53:A:VAL:HG11 | 1:60:A:TYR:HB3  | 11       | 0.15          |
| (1,717)  | 1:53:A:VAL:HG12 | 1:60:A:TYR:HB3  | 11       | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,717) | 1:53:A:VAL:HG13 | 1:60:A:TYR:HB3  | 11       | 0.15          |
| (1,717) | 1:53:A:VAL:HG21 | 1:60:A:TYR:HB3  | 11       | 0.15          |
| (1,717) | 1:53:A:VAL:HG22 | 1:60:A:TYR:HB3  | 11       | 0.15          |
| (1,717) | 1:53:A:VAL:HG23 | 1:60:A:TYR:HB3  | 11       | 0.15          |
| (1,717) | 1:53:A:VAL:HG11 | 1:60:A:TYR:HB3  | 19       | 0.15          |
| (1,717) | 1:53:A:VAL:HG12 | 1:60:A:TYR:HB3  | 19       | 0.15          |
| (1,717) | 1:53:A:VAL:HG13 | 1:60:A:TYR:HB3  | 19       | 0.15          |
| (1,717) | 1:53:A:VAL:HG21 | 1:60:A:TYR:HB3  | 19       | 0.15          |
| (1,717) | 1:53:A:VAL:HG22 | 1:60:A:TYR:HB3  | 19       | 0.15          |
| (1,717) | 1:53:A:VAL:HG23 | 1:60:A:TYR:HB3  | 19       | 0.15          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD21 | 10       | 0.15          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD22 | 10       | 0.15          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD23 | 10       | 0.15          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD21 | 12       | 0.15          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD22 | 12       | 0.15          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD23 | 12       | 0.15          |
| (1,689) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD11 | 6        | 0.15          |
| (1,689) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD12 | 6        | 0.15          |
| (1,689) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD13 | 6        | 0.15          |
| (1,689) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD11 | 9        | 0.15          |
| (1,689) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD12 | 9        | 0.15          |
| (1,689) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD13 | 9        | 0.15          |
| (1,625) | 1:8:A:ARG:HG2   | 1:59:A:PRO:HG2  | 10       | 0.15          |
| (1,625) | 1:8:A:ARG:HG3   | 1:59:A:PRO:HG2  | 10       | 0.15          |
| (1,625) | 1:8:A:ARG:HG2   | 1:59:A:PRO:HG2  | 20       | 0.15          |
| (1,625) | 1:8:A:ARG:HG3   | 1:59:A:PRO:HG2  | 20       | 0.15          |
| (1,599) | 1:37:A:LEU:HA   | 1:38:A:LEU:HB3  | 10       | 0.15          |
| (1,599) | 1:37:A:LEU:HA   | 1:38:A:LEU:HB3  | 20       | 0.15          |
| (1,590) | 1:13:A:PRO:HB3  | 1:46:A:ALA:HB1  | 12       | 0.15          |
| (1,590) | 1:13:A:PRO:HB3  | 1:46:A:ALA:HB2  | 12       | 0.15          |
| (1,590) | 1:13:A:PRO:HB3  | 1:46:A:ALA:HB3  | 12       | 0.15          |
| (1,575) | 1:10:A:ARG:HA   | 1:10:A:ARG:HG3  | 3        | 0.15          |
| (1,575) | 1:10:A:ARG:HA   | 1:10:A:ARG:HG3  | 6        | 0.15          |
| (1,556) | 1:29:A:GLU:HG2  | 1:60:A:TYR:HB2  | 19       | 0.15          |
| (1,556) | 1:29:A:GLU:HG3  | 1:60:A:TYR:HB2  | 19       | 0.15          |
| (1,547) | 1:8:A:ARG:HB2   | 1:59:A:PRO:HG3  | 4        | 0.15          |
| (1,547) | 1:8:A:ARG:HB3   | 1:59:A:PRO:HG3  | 4        | 0.15          |
| (1,538) | 1:18:A:GLU:HB3  | 1:19:A:LEU:H    | 2        | 0.15          |
| (1,505) | 1:41:A:GLU:HA   | 1:44:A:ASP:HB3  | 9        | 0.15          |
| (1,465) | 1:32:A:TYR:HE1  | 1:55:A:ARG:HG2  | 6        | 0.15          |
| (1,465) | 1:32:A:TYR:HE2  | 1:55:A:ARG:HG2  | 6        | 0.15          |
| (1,465) | 1:32:A:TYR:HE1  | 1:55:A:ARG:HG2  | 17       | 0.15          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,465) | 1:32:A:TYR:HE2 | 1:55:A:ARG:HG2  | 17       | 0.15          |
| (1,464) | 1:32:A:TYR:HA  | 1:32:A:TYR:HE1  | 7        | 0.15          |
| (1,464) | 1:32:A:TYR:HA  | 1:32:A:TYR:HE2  | 7        | 0.15          |
| (1,464) | 1:32:A:TYR:HA  | 1:32:A:TYR:HE1  | 13       | 0.15          |
| (1,464) | 1:32:A:TYR:HA  | 1:32:A:TYR:HE2  | 13       | 0.15          |
| (1,459) | 1:50:A:LEU:H   | 1:50:A:LEU:HG   | 5        | 0.15          |
| (1,409) | 1:78:A:HIS:HB2 | 1:78:A:HIS:HD2  | 15       | 0.15          |
| (1,401) | 1:32:A:TYR:HD1 | 1:55:A:ARG:HG2  | 8        | 0.15          |
| (1,401) | 1:32:A:TYR:HD2 | 1:55:A:ARG:HG2  | 8        | 0.15          |
| (1,401) | 1:32:A:TYR:HD1 | 1:55:A:ARG:HG2  | 10       | 0.15          |
| (1,401) | 1:32:A:TYR:HD2 | 1:55:A:ARG:HG2  | 10       | 0.15          |
| (1,382) | 1:78:A:HIS:HB3 | 1:79:A:TYR:HD1  | 1        | 0.15          |
| (1,382) | 1:78:A:HIS:HB3 | 1:79:A:TYR:HD2  | 1        | 0.15          |
| (1,381) | 1:78:A:HIS:HB2 | 1:79:A:TYR:HD1  | 20       | 0.15          |
| (1,381) | 1:78:A:HIS:HB2 | 1:79:A:TYR:HD2  | 20       | 0.15          |
| (1,348) | 1:66:A:CYS:HA  | 1:69:A:PHE:HZ   | 12       | 0.15          |
| (1,334) | 1:45:A:PHE:HD1 | 1:62:A:VAL:HG11 | 14       | 0.15          |
| (1,334) | 1:45:A:PHE:HD1 | 1:62:A:VAL:HG12 | 14       | 0.15          |
| (1,334) | 1:45:A:PHE:HD1 | 1:62:A:VAL:HG13 | 14       | 0.15          |
| (1,334) | 1:45:A:PHE:HD2 | 1:62:A:VAL:HG11 | 14       | 0.15          |
| (1,334) | 1:45:A:PHE:HD2 | 1:62:A:VAL:HG12 | 14       | 0.15          |
| (1,334) | 1:45:A:PHE:HD2 | 1:62:A:VAL:HG13 | 14       | 0.15          |
| (1,316) | 1:2:A:PHE:HD1  | 1:9:A:PRO:HD3   | 15       | 0.15          |
| (1,316) | 1:2:A:PHE:HD2  | 1:9:A:PRO:HD3   | 15       | 0.15          |
| (1,313) | 1:2:A:PHE:H    | 1:2:A:PHE:HD1   | 4        | 0.15          |
| (1,313) | 1:2:A:PHE:H    | 1:2:A:PHE:HD2   | 4        | 0.15          |
| (1,313) | 1:2:A:PHE:H    | 1:2:A:PHE:HD1   | 13       | 0.15          |
| (1,313) | 1:2:A:PHE:H    | 1:2:A:PHE:HD2   | 13       | 0.15          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD11 | 7        | 0.15          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD12 | 7        | 0.15          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD13 | 7        | 0.15          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD11 | 11       | 0.15          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD12 | 11       | 0.15          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD13 | 11       | 0.15          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD11 | 17       | 0.15          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD12 | 17       | 0.15          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD13 | 17       | 0.15          |
| (1,256) | 1:9:A:PRO:HB3  | 1:11:A:LYS:H    | 13       | 0.15          |
| (1,223) | 1:7:A:GLU:H    | 1:7:A:GLU:HB3   | 7        | 0.15          |
| (1,207) | 1:76:A:TYR:H   | 1:76:A:TYR:HD1  | 13       | 0.15          |
| (1,207) | 1:76:A:TYR:H   | 1:76:A:TYR:HD2  | 13       | 0.15          |
| (1,116) | 1:44:A:ASP:H   | 1:44:A:ASP:HB3  | 2        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,116)  | 1:44:A:ASP:H    | 1:44:A:ASP:HB3  | 5        | 0.15          |
| (1,116)  | 1:44:A:ASP:H    | 1:44:A:ASP:HB3  | 8        | 0.15          |
| (1,116)  | 1:44:A:ASP:H    | 1:44:A:ASP:HB3  | 19       | 0.15          |
| (1,96)   | 1:35:A:GLN:HB2  | 1:36:A:GLN:H    | 3        | 0.15          |
| (1,82)   | 1:54:A:TYR:H    | 1:59:A:PRO:HA   | 3        | 0.15          |
| (1,82)   | 1:54:A:TYR:H    | 1:59:A:PRO:HA   | 6        | 0.15          |
| (1,82)   | 1:54:A:TYR:H    | 1:59:A:PRO:HA   | 13       | 0.15          |
| (1,82)   | 1:54:A:TYR:H    | 1:59:A:PRO:HA   | 20       | 0.15          |
| (1,53)   | 1:37:A:LEU:H    | 1:37:A:LEU:HB3  | 5        | 0.15          |
| (1,53)   | 1:37:A:LEU:H    | 1:37:A:LEU:HB3  | 19       | 0.15          |
| (1,49)   | 1:55:A:ARG:H    | 1:59:A:PRO:HA   | 12       | 0.15          |
| (1,49)   | 1:55:A:ARG:H    | 1:59:A:PRO:HA   | 15       | 0.15          |
| (1,49)   | 1:55:A:ARG:H    | 1:59:A:PRO:HA   | 17       | 0.15          |
| (1,45)   | 1:36:A:GLN:HG3  | 1:37:A:LEU:H    | 7        | 0.15          |
| (1,26)   | 1:63:A:CYS:H    | 1:66:A:CYS:HB3  | 9        | 0.15          |
| (1,1244) | 1:30:A:CYS:H    | 1:63:A:CYS:H    | 15       | 0.14          |
| (1,1234) | 1:10:A:ARG:HA   | 1:52:A:ILE:HD11 | 6        | 0.14          |
| (1,1234) | 1:10:A:ARG:HA   | 1:52:A:ILE:HD12 | 6        | 0.14          |
| (1,1234) | 1:10:A:ARG:HA   | 1:52:A:ILE:HD13 | 6        | 0.14          |
| (1,1234) | 1:10:A:ARG:HA   | 1:52:A:ILE:HD11 | 16       | 0.14          |
| (1,1234) | 1:10:A:ARG:HA   | 1:52:A:ILE:HD12 | 16       | 0.14          |
| (1,1234) | 1:10:A:ARG:HA   | 1:52:A:ILE:HD13 | 16       | 0.14          |
| (1,1229) | 1:55:A:ARG:HG3  | 1:32:A:TYR:H    | 15       | 0.14          |
| (1,1228) | 1:9:A:PRO:HG2   | 1:54:A:TYR:HE1  | 16       | 0.14          |
| (1,1228) | 1:9:A:PRO:HG2   | 1:54:A:TYR:HE2  | 16       | 0.14          |
| (1,1228) | 1:9:A:PRO:HG3   | 1:54:A:TYR:HE1  | 16       | 0.14          |
| (1,1228) | 1:9:A:PRO:HG3   | 1:54:A:TYR:HE2  | 16       | 0.14          |
| (1,1225) | 1:2:A:PHE:HE1   | 1:54:A:TYR:HE1  | 14       | 0.14          |
| (1,1225) | 1:2:A:PHE:HE1   | 1:54:A:TYR:HE2  | 14       | 0.14          |
| (1,1225) | 1:2:A:PHE:HE2   | 1:54:A:TYR:HE1  | 14       | 0.14          |
| (1,1225) | 1:2:A:PHE:HE2   | 1:54:A:TYR:HE2  | 14       | 0.14          |
| (1,1170) | 1:48:A:ARG:H    | 1:48:A:ARG:HD3  | 4        | 0.14          |
| (1,1170) | 1:48:A:ARG:H    | 1:48:A:ARG:HD3  | 7        | 0.14          |
| (1,1163) | 1:4:A:ASP:HA    | 1:6:A:GLN:H     | 15       | 0.14          |
| (1,1118) | 1:7:A:GLU:HA    | 1:8:A:ARG:H     | 3        | 0.14          |
| (1,1114) | 1:36:A:GLN:H    | 1:36:A:GLN:HG3  | 2        | 0.14          |
| (1,1108) | 1:52:A:ILE:HD11 | 1:61:A:ALA:H    | 3        | 0.14          |
| (1,1108) | 1:52:A:ILE:HD12 | 1:61:A:ALA:H    | 3        | 0.14          |
| (1,1108) | 1:52:A:ILE:HD13 | 1:61:A:ALA:H    | 3        | 0.14          |
| (1,1108) | 1:52:A:ILE:HD11 | 1:61:A:ALA:H    | 10       | 0.14          |
| (1,1108) | 1:52:A:ILE:HD12 | 1:61:A:ALA:H    | 10       | 0.14          |
| (1,1108) | 1:52:A:ILE:HD13 | 1:61:A:ALA:H    | 10       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1108) | 1:52:A:ILE:HD11 | 1:61:A:ALA:H    | 15       | 0.14          |
| (1,1108) | 1:52:A:ILE:HD12 | 1:61:A:ALA:H    | 15       | 0.14          |
| (1,1108) | 1:52:A:ILE:HD13 | 1:61:A:ALA:H    | 15       | 0.14          |
| (1,1099) | 1:77:A:ARG:H    | 1:78:A:HIS:HB3  | 15       | 0.14          |
| (1,1057) | 1:1:A:MET:HE1   | 1:2:A:PHE:HA    | 9        | 0.14          |
| (1,1057) | 1:1:A:MET:HE2   | 1:2:A:PHE:HA    | 9        | 0.14          |
| (1,1057) | 1:1:A:MET:HE3   | 1:2:A:PHE:HA    | 9        | 0.14          |
| (1,1035) | 1:17:A:THR:HG21 | 1:18:A:GLU:HG3  | 5        | 0.14          |
| (1,1035) | 1:17:A:THR:HG22 | 1:18:A:GLU:HG3  | 5        | 0.14          |
| (1,1035) | 1:17:A:THR:HG23 | 1:18:A:GLU:HG3  | 5        | 0.14          |
| (1,1035) | 1:17:A:THR:HG21 | 1:18:A:GLU:HG3  | 6        | 0.14          |
| (1,1035) | 1:17:A:THR:HG22 | 1:18:A:GLU:HG3  | 6        | 0.14          |
| (1,1035) | 1:17:A:THR:HG23 | 1:18:A:GLU:HG3  | 6        | 0.14          |
| (1,1035) | 1:17:A:THR:HG21 | 1:18:A:GLU:HG3  | 7        | 0.14          |
| (1,1035) | 1:17:A:THR:HG22 | 1:18:A:GLU:HG3  | 7        | 0.14          |
| (1,1035) | 1:17:A:THR:HG23 | 1:18:A:GLU:HG3  | 7        | 0.14          |
| (1,1035) | 1:17:A:THR:HG21 | 1:18:A:GLU:HG3  | 8        | 0.14          |
| (1,1035) | 1:17:A:THR:HG22 | 1:18:A:GLU:HG3  | 8        | 0.14          |
| (1,1035) | 1:17:A:THR:HG23 | 1:18:A:GLU:HG3  | 8        | 0.14          |
| (1,1035) | 1:17:A:THR:HG21 | 1:18:A:GLU:HG3  | 9        | 0.14          |
| (1,1035) | 1:17:A:THR:HG22 | 1:18:A:GLU:HG3  | 9        | 0.14          |
| (1,1035) | 1:17:A:THR:HG23 | 1:18:A:GLU:HG3  | 9        | 0.14          |
| (1,1035) | 1:17:A:THR:HG21 | 1:18:A:GLU:HG3  | 12       | 0.14          |
| (1,1035) | 1:17:A:THR:HG22 | 1:18:A:GLU:HG3  | 12       | 0.14          |
| (1,1035) | 1:17:A:THR:HG23 | 1:18:A:GLU:HG3  | 12       | 0.14          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG11 | 9        | 0.14          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG12 | 9        | 0.14          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG13 | 9        | 0.14          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG11 | 18       | 0.14          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG12 | 18       | 0.14          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG13 | 18       | 0.14          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD21 | 8        | 0.14          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD22 | 8        | 0.14          |
| (1,1018) | 1:15:A:LEU:H    | 1:15:A:LEU:HD23 | 8        | 0.14          |
| (1,996)  | 1:10:A:ARG:HA   | 1:10:A:ARG:HG2  | 20       | 0.14          |
| (1,984)  | 1:26:A:ILE:HG13 | 1:28:A:LEU:HA   | 4        | 0.14          |
| (1,984)  | 1:26:A:ILE:HG13 | 1:28:A:LEU:HA   | 10       | 0.14          |
| (1,984)  | 1:26:A:ILE:HG13 | 1:28:A:LEU:HA   | 19       | 0.14          |
| (1,964)  | 1:53:A:VAL:HG21 | 1:62:A:VAL:HB   | 4        | 0.14          |
| (1,964)  | 1:53:A:VAL:HG22 | 1:62:A:VAL:HB   | 4        | 0.14          |
| (1,964)  | 1:53:A:VAL:HG23 | 1:62:A:VAL:HB   | 4        | 0.14          |
| (1,956)  | 1:18:A:GLU:H    | 1:18:A:GLU:HG2  | 1        | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,867) | 1:15:A:LEU:HD11 | 1:18:A:GLU:HA   | 2        | 0.14          |
| (1,867) | 1:15:A:LEU:HD12 | 1:18:A:GLU:HA   | 2        | 0.14          |
| (1,867) | 1:15:A:LEU:HD13 | 1:18:A:GLU:HA   | 2        | 0.14          |
| (1,867) | 1:15:A:LEU:HD11 | 1:18:A:GLU:HA   | 3        | 0.14          |
| (1,867) | 1:15:A:LEU:HD12 | 1:18:A:GLU:HA   | 3        | 0.14          |
| (1,867) | 1:15:A:LEU:HD13 | 1:18:A:GLU:HA   | 3        | 0.14          |
| (1,867) | 1:15:A:LEU:HD11 | 1:18:A:GLU:HA   | 16       | 0.14          |
| (1,867) | 1:15:A:LEU:HD12 | 1:18:A:GLU:HA   | 16       | 0.14          |
| (1,867) | 1:15:A:LEU:HD13 | 1:18:A:GLU:HA   | 16       | 0.14          |
| (1,864) | 1:69:A:PHE:HA   | 1:69:A:PHE:HB2  | 3        | 0.14          |
| (1,864) | 1:69:A:PHE:HA   | 1:69:A:PHE:HB2  | 16       | 0.14          |
| (1,850) | 1:23:A:ILE:HA   | 1:23:A:ILE:HG13 | 1        | 0.14          |
| (1,850) | 1:23:A:ILE:HA   | 1:23:A:ILE:HG13 | 2        | 0.14          |
| (1,850) | 1:23:A:ILE:HA   | 1:23:A:ILE:HG13 | 7        | 0.14          |
| (1,850) | 1:23:A:ILE:HA   | 1:23:A:ILE:HG13 | 8        | 0.14          |
| (1,717) | 1:53:A:VAL:HG11 | 1:60:A:TYR:HB3  | 2        | 0.14          |
| (1,717) | 1:53:A:VAL:HG12 | 1:60:A:TYR:HB3  | 2        | 0.14          |
| (1,717) | 1:53:A:VAL:HG13 | 1:60:A:TYR:HB3  | 2        | 0.14          |
| (1,717) | 1:53:A:VAL:HG21 | 1:60:A:TYR:HB3  | 2        | 0.14          |
| (1,717) | 1:53:A:VAL:HG22 | 1:60:A:TYR:HB3  | 2        | 0.14          |
| (1,717) | 1:53:A:VAL:HG23 | 1:60:A:TYR:HB3  | 2        | 0.14          |
| (1,717) | 1:53:A:VAL:HG11 | 1:60:A:TYR:HB3  | 7        | 0.14          |
| (1,717) | 1:53:A:VAL:HG12 | 1:60:A:TYR:HB3  | 7        | 0.14          |
| (1,717) | 1:53:A:VAL:HG13 | 1:60:A:TYR:HB3  | 7        | 0.14          |
| (1,717) | 1:53:A:VAL:HG21 | 1:60:A:TYR:HB3  | 7        | 0.14          |
| (1,717) | 1:53:A:VAL:HG22 | 1:60:A:TYR:HB3  | 7        | 0.14          |
| (1,717) | 1:53:A:VAL:HG23 | 1:60:A:TYR:HB3  | 7        | 0.14          |
| (1,717) | 1:53:A:VAL:HG11 | 1:60:A:TYR:HB3  | 9        | 0.14          |
| (1,717) | 1:53:A:VAL:HG12 | 1:60:A:TYR:HB3  | 9        | 0.14          |
| (1,717) | 1:53:A:VAL:HG13 | 1:60:A:TYR:HB3  | 9        | 0.14          |
| (1,717) | 1:53:A:VAL:HG21 | 1:60:A:TYR:HB3  | 9        | 0.14          |
| (1,717) | 1:53:A:VAL:HG22 | 1:60:A:TYR:HB3  | 9        | 0.14          |
| (1,717) | 1:53:A:VAL:HG23 | 1:60:A:TYR:HB3  | 9        | 0.14          |
| (1,717) | 1:53:A:VAL:HG11 | 1:60:A:TYR:HB3  | 15       | 0.14          |
| (1,717) | 1:53:A:VAL:HG12 | 1:60:A:TYR:HB3  | 15       | 0.14          |
| (1,717) | 1:53:A:VAL:HG13 | 1:60:A:TYR:HB3  | 15       | 0.14          |
| (1,717) | 1:53:A:VAL:HG21 | 1:60:A:TYR:HB3  | 15       | 0.14          |
| (1,717) | 1:53:A:VAL:HG22 | 1:60:A:TYR:HB3  | 15       | 0.14          |
| (1,717) | 1:53:A:VAL:HG23 | 1:60:A:TYR:HB3  | 15       | 0.14          |
| (1,717) | 1:53:A:VAL:HG11 | 1:60:A:TYR:HB3  | 20       | 0.14          |
| (1,717) | 1:53:A:VAL:HG12 | 1:60:A:TYR:HB3  | 20       | 0.14          |
| (1,717) | 1:53:A:VAL:HG13 | 1:60:A:TYR:HB3  | 20       | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,717) | 1:53:A:VAL:HG21 | 1:60:A:TYR:HB3  | 20       | 0.14          |
| (1,717) | 1:53:A:VAL:HG22 | 1:60:A:TYR:HB3  | 20       | 0.14          |
| (1,717) | 1:53:A:VAL:HG23 | 1:60:A:TYR:HB3  | 20       | 0.14          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD21 | 3        | 0.14          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD22 | 3        | 0.14          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD23 | 3        | 0.14          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD21 | 16       | 0.14          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD22 | 16       | 0.14          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD23 | 16       | 0.14          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD21 | 18       | 0.14          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD22 | 18       | 0.14          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD23 | 18       | 0.14          |
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD11 | 6        | 0.14          |
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD12 | 6        | 0.14          |
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD13 | 6        | 0.14          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD11 | 6        | 0.14          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD12 | 6        | 0.14          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD13 | 6        | 0.14          |
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD11 | 6        | 0.14          |
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD12 | 6        | 0.14          |
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD13 | 6        | 0.14          |
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD11 | 8        | 0.14          |
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD12 | 8        | 0.14          |
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD13 | 8        | 0.14          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD11 | 8        | 0.14          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD12 | 8        | 0.14          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD13 | 8        | 0.14          |
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD11 | 8        | 0.14          |
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD12 | 8        | 0.14          |
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD13 | 8        | 0.14          |
| (1,649) | 1:52:A:ILE:HA   | 1:62:A:VAL:HG21 | 13       | 0.14          |
| (1,649) | 1:52:A:ILE:HA   | 1:62:A:VAL:HG22 | 13       | 0.14          |
| (1,649) | 1:52:A:ILE:HA   | 1:62:A:VAL:HG23 | 13       | 0.14          |
| (1,628) | 1:34:A:LYS:H    | 1:34:A:LYS:HG2  | 2        | 0.14          |
| (1,628) | 1:34:A:LYS:H    | 1:34:A:LYS:HG2  | 5        | 0.14          |
| (1,625) | 1:8:A:ARG:HG2   | 1:59:A:PRO:HG2  | 5        | 0.14          |
| (1,625) | 1:8:A:ARG:HG3   | 1:59:A:PRO:HG2  | 5        | 0.14          |
| (1,625) | 1:8:A:ARG:HG2   | 1:59:A:PRO:HG2  | 18       | 0.14          |
| (1,625) | 1:8:A:ARG:HG3   | 1:59:A:PRO:HG2  | 18       | 0.14          |
| (1,599) | 1:37:A:LEU:HA   | 1:38:A:LEU:HB3  | 2        | 0.14          |
| (1,595) | 1:16:A:CYS:HA   | 1:19:A:LEU:HB3  | 16       | 0.14          |
| (1,590) | 1:13:A:PRO:HB3  | 1:46:A:ALA:HB1  | 14       | 0.14          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,590) | 1:13:A:PRO:HB3 | 1:46:A:ALA:HB2 | 14       | 0.14          |
| (1,590) | 1:13:A:PRO:HB3 | 1:46:A:ALA:HB3 | 14       | 0.14          |
| (1,590) | 1:13:A:PRO:HB3 | 1:46:A:ALA:HB1 | 16       | 0.14          |
| (1,590) | 1:13:A:PRO:HB3 | 1:46:A:ALA:HB2 | 16       | 0.14          |
| (1,590) | 1:13:A:PRO:HB3 | 1:46:A:ALA:HB3 | 16       | 0.14          |
| (1,578) | 1:67:A:LEU:H   | 1:67:A:LEU:HG  | 1        | 0.14          |
| (1,575) | 1:10:A:ARG:HA  | 1:10:A:ARG:HG3 | 10       | 0.14          |
| (1,575) | 1:10:A:ARG:HA  | 1:10:A:ARG:HG3 | 16       | 0.14          |
| (1,574) | 1:11:A:LYS:HA  | 1:11:A:LYS:HD2 | 4        | 0.14          |
| (1,574) | 1:11:A:LYS:HA  | 1:11:A:LYS:HD3 | 4        | 0.14          |
| (1,574) | 1:11:A:LYS:HA  | 1:11:A:LYS:HD2 | 19       | 0.14          |
| (1,574) | 1:11:A:LYS:HA  | 1:11:A:LYS:HD3 | 19       | 0.14          |
| (1,561) | 1:39:A:ARG:HG2 | 1:43:A:TYR:HB2 | 15       | 0.14          |
| (1,561) | 1:39:A:ARG:HG2 | 1:43:A:TYR:HB3 | 15       | 0.14          |
| (1,561) | 1:39:A:ARG:HG3 | 1:43:A:TYR:HB2 | 15       | 0.14          |
| (1,561) | 1:39:A:ARG:HG3 | 1:43:A:TYR:HB3 | 15       | 0.14          |
| (1,561) | 1:39:A:ARG:HG2 | 1:43:A:TYR:HB2 | 20       | 0.14          |
| (1,561) | 1:39:A:ARG:HG2 | 1:43:A:TYR:HB3 | 20       | 0.14          |
| (1,561) | 1:39:A:ARG:HG3 | 1:43:A:TYR:HB2 | 20       | 0.14          |
| (1,561) | 1:39:A:ARG:HG3 | 1:43:A:TYR:HB3 | 20       | 0.14          |
| (1,556) | 1:29:A:GLU:HG2 | 1:60:A:TYR:HB2 | 10       | 0.14          |
| (1,556) | 1:29:A:GLU:HG3 | 1:60:A:TYR:HB2 | 10       | 0.14          |
| (1,538) | 1:18:A:GLU:HB3 | 1:19:A:LEU:H   | 10       | 0.14          |
| (1,480) | 1:46:A:ALA:H   | 1:47:A:ARG:HD2 | 3        | 0.14          |
| (1,480) | 1:46:A:ALA:H   | 1:47:A:ARG:HD3 | 3        | 0.14          |
| (1,478) | 1:8:A:ARG:HG2  | 1:59:A:PRO:HD2 | 20       | 0.14          |
| (1,478) | 1:8:A:ARG:HG3  | 1:59:A:PRO:HD2 | 20       | 0.14          |
| (1,477) | 1:77:A:ARG:H   | 1:78:A:HIS:HA  | 2        | 0.14          |
| (1,467) | 1:54:A:TYR:HE1 | 1:58:A:ASN:HA  | 8        | 0.14          |
| (1,467) | 1:54:A:TYR:HE2 | 1:58:A:ASN:HA  | 8        | 0.14          |
| (1,467) | 1:54:A:TYR:HE1 | 1:58:A:ASN:HA  | 12       | 0.14          |
| (1,467) | 1:54:A:TYR:HE2 | 1:58:A:ASN:HA  | 12       | 0.14          |
| (1,467) | 1:54:A:TYR:HE1 | 1:58:A:ASN:HA  | 16       | 0.14          |
| (1,467) | 1:54:A:TYR:HE2 | 1:58:A:ASN:HA  | 16       | 0.14          |
| (1,465) | 1:32:A:TYR:HE1 | 1:55:A:ARG:HG2 | 1        | 0.14          |
| (1,465) | 1:32:A:TYR:HE2 | 1:55:A:ARG:HG2 | 1        | 0.14          |
| (1,465) | 1:32:A:TYR:HE1 | 1:55:A:ARG:HG2 | 10       | 0.14          |
| (1,465) | 1:32:A:TYR:HE2 | 1:55:A:ARG:HG2 | 10       | 0.14          |
| (1,465) | 1:32:A:TYR:HE1 | 1:55:A:ARG:HG2 | 19       | 0.14          |
| (1,465) | 1:32:A:TYR:HE2 | 1:55:A:ARG:HG2 | 19       | 0.14          |
| (1,464) | 1:32:A:TYR:HA  | 1:32:A:TYR:HE1 | 5        | 0.14          |
| (1,464) | 1:32:A:TYR:HA  | 1:32:A:TYR:HE2 | 5        | 0.14          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,459) | 1:50:A:LEU:H   | 1:50:A:LEU:HG   | 9        | 0.14          |
| (1,459) | 1:50:A:LEU:H   | 1:50:A:LEU:HG   | 13       | 0.14          |
| (1,459) | 1:50:A:LEU:H   | 1:50:A:LEU:HG   | 14       | 0.14          |
| (1,430) | 1:3:A:GLN:HA   | 1:3:A:GLN:HE22  | 20       | 0.14          |
| (1,418) | 1:29:A:GLU:HG2 | 1:60:A:TYR:HD1  | 4        | 0.14          |
| (1,418) | 1:29:A:GLU:HG2 | 1:60:A:TYR:HD2  | 4        | 0.14          |
| (1,418) | 1:29:A:GLU:HG3 | 1:60:A:TYR:HD1  | 4        | 0.14          |
| (1,418) | 1:29:A:GLU:HG3 | 1:60:A:TYR:HD2  | 4        | 0.14          |
| (1,408) | 1:78:A:HIS:HA  | 1:78:A:HIS:HD2  | 8        | 0.14          |
| (1,401) | 1:32:A:TYR:HD1 | 1:55:A:ARG:HG2  | 7        | 0.14          |
| (1,401) | 1:32:A:TYR:HD2 | 1:55:A:ARG:HG2  | 7        | 0.14          |
| (1,401) | 1:32:A:TYR:HD1 | 1:55:A:ARG:HG2  | 9        | 0.14          |
| (1,401) | 1:32:A:TYR:HD2 | 1:55:A:ARG:HG2  | 9        | 0.14          |
| (1,401) | 1:32:A:TYR:HD1 | 1:55:A:ARG:HG2  | 19       | 0.14          |
| (1,401) | 1:32:A:TYR:HD2 | 1:55:A:ARG:HG2  | 19       | 0.14          |
| (1,381) | 1:78:A:HIS:HB2 | 1:79:A:TYR:HD1  | 13       | 0.14          |
| (1,381) | 1:78:A:HIS:HB2 | 1:79:A:TYR:HD2  | 13       | 0.14          |
| (1,334) | 1:45:A:PHE:HD1 | 1:62:A:VAL:HG11 | 12       | 0.14          |
| (1,334) | 1:45:A:PHE:HD1 | 1:62:A:VAL:HG12 | 12       | 0.14          |
| (1,334) | 1:45:A:PHE:HD1 | 1:62:A:VAL:HG13 | 12       | 0.14          |
| (1,334) | 1:45:A:PHE:HD2 | 1:62:A:VAL:HG11 | 12       | 0.14          |
| (1,334) | 1:45:A:PHE:HD2 | 1:62:A:VAL:HG12 | 12       | 0.14          |
| (1,334) | 1:45:A:PHE:HD2 | 1:62:A:VAL:HG13 | 12       | 0.14          |
| (1,316) | 1:2:A:PHE:HD1  | 1:9:A:PRO:HD3   | 7        | 0.14          |
| (1,316) | 1:2:A:PHE:HD2  | 1:9:A:PRO:HD3   | 7        | 0.14          |
| (1,313) | 1:2:A:PHE:H    | 1:2:A:PHE:HD1   | 1        | 0.14          |
| (1,313) | 1:2:A:PHE:H    | 1:2:A:PHE:HD2   | 1        | 0.14          |
| (1,313) | 1:2:A:PHE:H    | 1:2:A:PHE:HD1   | 5        | 0.14          |
| (1,313) | 1:2:A:PHE:H    | 1:2:A:PHE:HD2   | 5        | 0.14          |
| (1,310) | 1:2:A:PHE:HD1  | 1:8:A:ARG:H     | 8        | 0.14          |
| (1,310) | 1:2:A:PHE:HD2  | 1:8:A:ARG:H     | 8        | 0.14          |
| (1,310) | 1:2:A:PHE:HD1  | 1:8:A:ARG:H     | 12       | 0.14          |
| (1,310) | 1:2:A:PHE:HD2  | 1:8:A:ARG:H     | 12       | 0.14          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD11 | 12       | 0.14          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD12 | 12       | 0.14          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD13 | 12       | 0.14          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD11 | 19       | 0.14          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD12 | 19       | 0.14          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD13 | 19       | 0.14          |
| (1,292) | 1:2:A:PHE:HA   | 1:2:A:PHE:HE1   | 18       | 0.14          |
| (1,292) | 1:2:A:PHE:HA   | 1:2:A:PHE:HE2   | 18       | 0.14          |
| (1,256) | 1:9:A:PRO:HB3  | 1:11:A:LYS:H    | 3        | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,256)  | 1:9:A:PRO:HB3   | 1:11:A:LYS:H    | 15       | 0.14          |
| (1,239)  | 1:11:A:LYS:HD2  | 1:14:A:GLN:HE21 | 18       | 0.14          |
| (1,239)  | 1:11:A:LYS:HD3  | 1:14:A:GLN:HE21 | 18       | 0.14          |
| (1,226)  | 1:7:A:GLU:H     | 1:7:A:GLU:HG2   | 7        | 0.14          |
| (1,116)  | 1:44:A:ASP:H    | 1:44:A:ASP:HB3  | 9        | 0.14          |
| (1,116)  | 1:44:A:ASP:H    | 1:44:A:ASP:HB3  | 11       | 0.14          |
| (1,116)  | 1:44:A:ASP:H    | 1:44:A:ASP:HB3  | 14       | 0.14          |
| (1,116)  | 1:44:A:ASP:H    | 1:44:A:ASP:HB3  | 18       | 0.14          |
| (1,82)   | 1:54:A:TYR:H    | 1:59:A:PRO:HA   | 5        | 0.14          |
| (1,82)   | 1:54:A:TYR:H    | 1:59:A:PRO:HA   | 19       | 0.14          |
| (1,49)   | 1:55:A:ARG:H    | 1:59:A:PRO:HA   | 9        | 0.14          |
| (1,49)   | 1:55:A:ARG:H    | 1:59:A:PRO:HA   | 19       | 0.14          |
| (1,1242) | 1:29:A:GLU:HB2  | 1:60:A:TYR:HB2  | 16       | 0.13          |
| (1,1240) | 1:41:A:GLU:HG2  | 1:64:A:ASP:HB2  | 18       | 0.13          |
| (1,1234) | 1:10:A:ARG:HA   | 1:52:A:ILE:HD11 | 1        | 0.13          |
| (1,1234) | 1:10:A:ARG:HA   | 1:52:A:ILE:HD12 | 1        | 0.13          |
| (1,1234) | 1:10:A:ARG:HA   | 1:52:A:ILE:HD13 | 1        | 0.13          |
| (1,1225) | 1:2:A:PHE:HE1   | 1:54:A:TYR:HE1  | 4        | 0.13          |
| (1,1225) | 1:2:A:PHE:HE1   | 1:54:A:TYR:HE2  | 4        | 0.13          |
| (1,1225) | 1:2:A:PHE:HE2   | 1:54:A:TYR:HE1  | 4        | 0.13          |
| (1,1225) | 1:2:A:PHE:HE2   | 1:54:A:TYR:HE2  | 4        | 0.13          |
| (1,1225) | 1:2:A:PHE:HE1   | 1:54:A:TYR:HE1  | 18       | 0.13          |
| (1,1225) | 1:2:A:PHE:HE1   | 1:54:A:TYR:HE2  | 18       | 0.13          |
| (1,1225) | 1:2:A:PHE:HE2   | 1:54:A:TYR:HE1  | 18       | 0.13          |
| (1,1225) | 1:2:A:PHE:HE2   | 1:54:A:TYR:HE2  | 18       | 0.13          |
| (1,1218) | 1:3:A:GLN:HE21  | 1:4:A:ASP:HA    | 9        | 0.13          |
| (1,1215) | 1:3:A:GLN:HE22  | 1:4:A:ASP:HA    | 2        | 0.13          |
| (1,1177) | 1:19:A:LEU:H    | 1:19:A:LEU:HG   | 4        | 0.13          |
| (1,1170) | 1:48:A:ARG:H    | 1:48:A:ARG:HD3  | 11       | 0.13          |
| (1,1152) | 1:70:A:TYR:H    | 1:70:A:TYR:HB3  | 9        | 0.13          |
| (1,1140) | 1:29:A:GLU:H    | 1:29:A:GLU:HB2  | 3        | 0.13          |
| (1,1140) | 1:29:A:GLU:H    | 1:29:A:GLU:HB2  | 15       | 0.13          |
| (1,1118) | 1:7:A:GLU:HA    | 1:8:A:ARG:H     | 15       | 0.13          |
| (1,1118) | 1:7:A:GLU:HA    | 1:8:A:ARG:H     | 17       | 0.13          |
| (1,1114) | 1:36:A:GLN:H    | 1:36:A:GLN:HG3  | 19       | 0.13          |
| (1,1108) | 1:52:A:ILE:HD11 | 1:61:A:ALA:H    | 17       | 0.13          |
| (1,1108) | 1:52:A:ILE:HD12 | 1:61:A:ALA:H    | 17       | 0.13          |
| (1,1108) | 1:52:A:ILE:HD13 | 1:61:A:ALA:H    | 17       | 0.13          |
| (1,1108) | 1:52:A:ILE:HD11 | 1:61:A:ALA:H    | 19       | 0.13          |
| (1,1108) | 1:52:A:ILE:HD12 | 1:61:A:ALA:H    | 19       | 0.13          |
| (1,1108) | 1:52:A:ILE:HD13 | 1:61:A:ALA:H    | 19       | 0.13          |
| (1,1106) | 1:10:A:ARG:H    | 1:10:A:ARG:HB3  | 2        | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1099) | 1:77:A:ARG:H    | 1:78:A:HIS:HB3  | 4        | 0.13          |
| (1,1099) | 1:77:A:ARG:H    | 1:78:A:HIS:HB3  | 10       | 0.13          |
| (1,1072) | 1:29:A:GLU:HB2  | 1:37:A:LEU:H    | 4        | 0.13          |
| (1,1072) | 1:29:A:GLU:HB2  | 1:37:A:LEU:H    | 20       | 0.13          |
| (1,1057) | 1:1:A:MET:HE1   | 1:2:A:PHE:HA    | 11       | 0.13          |
| (1,1057) | 1:1:A:MET:HE2   | 1:2:A:PHE:HA    | 11       | 0.13          |
| (1,1057) | 1:1:A:MET:HE3   | 1:2:A:PHE:HA    | 11       | 0.13          |
| (1,1057) | 1:1:A:MET:HE1   | 1:2:A:PHE:HA    | 19       | 0.13          |
| (1,1057) | 1:1:A:MET:HE2   | 1:2:A:PHE:HA    | 19       | 0.13          |
| (1,1057) | 1:1:A:MET:HE3   | 1:2:A:PHE:HA    | 19       | 0.13          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB1  | 13       | 0.13          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB2  | 13       | 0.13          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB3  | 13       | 0.13          |
| (1,1035) | 1:17:A:THR:HG21 | 1:18:A:GLU:HG3  | 10       | 0.13          |
| (1,1035) | 1:17:A:THR:HG22 | 1:18:A:GLU:HG3  | 10       | 0.13          |
| (1,1035) | 1:17:A:THR:HG23 | 1:18:A:GLU:HG3  | 10       | 0.13          |
| (1,1035) | 1:17:A:THR:HG21 | 1:18:A:GLU:HG3  | 11       | 0.13          |
| (1,1035) | 1:17:A:THR:HG22 | 1:18:A:GLU:HG3  | 11       | 0.13          |
| (1,1035) | 1:17:A:THR:HG23 | 1:18:A:GLU:HG3  | 11       | 0.13          |
| (1,1035) | 1:17:A:THR:HG21 | 1:18:A:GLU:HG3  | 13       | 0.13          |
| (1,1035) | 1:17:A:THR:HG22 | 1:18:A:GLU:HG3  | 13       | 0.13          |
| (1,1035) | 1:17:A:THR:HG23 | 1:18:A:GLU:HG3  | 13       | 0.13          |
| (1,1035) | 1:17:A:THR:HG21 | 1:18:A:GLU:HG3  | 15       | 0.13          |
| (1,1035) | 1:17:A:THR:HG22 | 1:18:A:GLU:HG3  | 15       | 0.13          |
| (1,1035) | 1:17:A:THR:HG23 | 1:18:A:GLU:HG3  | 15       | 0.13          |
| (1,1035) | 1:17:A:THR:HG21 | 1:18:A:GLU:HG3  | 19       | 0.13          |
| (1,1035) | 1:17:A:THR:HG22 | 1:18:A:GLU:HG3  | 19       | 0.13          |
| (1,1035) | 1:17:A:THR:HG23 | 1:18:A:GLU:HG3  | 19       | 0.13          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG11 | 4        | 0.13          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG12 | 4        | 0.13          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG13 | 4        | 0.13          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG11 | 12       | 0.13          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG12 | 12       | 0.13          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG13 | 12       | 0.13          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG11 | 13       | 0.13          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG12 | 13       | 0.13          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG13 | 13       | 0.13          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG11 | 17       | 0.13          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG12 | 17       | 0.13          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG13 | 17       | 0.13          |
| (1,984)  | 1:26:A:ILE:HG13 | 1:28:A:LEU:HA   | 13       | 0.13          |
| (1,964)  | 1:53:A:VAL:HG21 | 1:62:A:VAL:HB   | 1        | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,964) | 1:53:A:VAL:HG22 | 1:62:A:VAL:HB   | 1        | 0.13          |
| (1,964) | 1:53:A:VAL:HG23 | 1:62:A:VAL:HB   | 1        | 0.13          |
| (1,964) | 1:53:A:VAL:HG21 | 1:62:A:VAL:HB   | 10       | 0.13          |
| (1,964) | 1:53:A:VAL:HG22 | 1:62:A:VAL:HB   | 10       | 0.13          |
| (1,964) | 1:53:A:VAL:HG23 | 1:62:A:VAL:HB   | 10       | 0.13          |
| (1,924) | 1:9:A:PRO:HD2   | 1:15:A:LEU:HB3  | 3        | 0.13          |
| (1,924) | 1:9:A:PRO:HD2   | 1:15:A:LEU:HB3  | 5        | 0.13          |
| (1,924) | 1:9:A:PRO:HD2   | 1:15:A:LEU:HB3  | 7        | 0.13          |
| (1,914) | 1:8:A:ARG:HA    | 1:9:A:PRO:HD2   | 8        | 0.13          |
| (1,907) | 1:77:A:ARG:HA   | 1:77:A:ARG:HG2  | 20       | 0.13          |
| (1,907) | 1:77:A:ARG:HA   | 1:77:A:ARG:HG3  | 20       | 0.13          |
| (1,888) | 1:44:A:ASP:HA   | 1:47:A:ARG:H    | 19       | 0.13          |
| (1,888) | 1:44:A:ASP:HA   | 1:47:A:ARG:H    | 20       | 0.13          |
| (1,872) | 1:73:A:ILE:HB   | 1:74:A:SER:HA   | 2        | 0.13          |
| (1,867) | 1:15:A:LEU:HD11 | 1:18:A:GLU:HA   | 17       | 0.13          |
| (1,867) | 1:15:A:LEU:HD12 | 1:18:A:GLU:HA   | 17       | 0.13          |
| (1,867) | 1:15:A:LEU:HD13 | 1:18:A:GLU:HA   | 17       | 0.13          |
| (1,864) | 1:69:A:PHE:HA   | 1:69:A:PHE:HB2  | 2        | 0.13          |
| (1,864) | 1:69:A:PHE:HA   | 1:69:A:PHE:HB2  | 4        | 0.13          |
| (1,864) | 1:69:A:PHE:HA   | 1:69:A:PHE:HB2  | 10       | 0.13          |
| (1,864) | 1:69:A:PHE:HA   | 1:69:A:PHE:HB2  | 11       | 0.13          |
| (1,864) | 1:69:A:PHE:HA   | 1:69:A:PHE:HB2  | 15       | 0.13          |
| (1,864) | 1:69:A:PHE:HA   | 1:69:A:PHE:HB2  | 17       | 0.13          |
| (1,850) | 1:23:A:ILE:HA   | 1:23:A:ILE:HG13 | 9        | 0.13          |
| (1,850) | 1:23:A:ILE:HA   | 1:23:A:ILE:HG13 | 12       | 0.13          |
| (1,850) | 1:23:A:ILE:HA   | 1:23:A:ILE:HG13 | 13       | 0.13          |
| (1,850) | 1:23:A:ILE:HA   | 1:23:A:ILE:HG13 | 14       | 0.13          |
| (1,850) | 1:23:A:ILE:HA   | 1:23:A:ILE:HG13 | 15       | 0.13          |
| (1,850) | 1:23:A:ILE:HA   | 1:23:A:ILE:HG13 | 16       | 0.13          |
| (1,850) | 1:23:A:ILE:HA   | 1:23:A:ILE:HG13 | 17       | 0.13          |
| (1,850) | 1:23:A:ILE:HA   | 1:23:A:ILE:HG13 | 19       | 0.13          |
| (1,850) | 1:23:A:ILE:HA   | 1:23:A:ILE:HG13 | 20       | 0.13          |
| (1,753) | 1:50:A:LEU:H    | 1:50:A:LEU:HD21 | 16       | 0.13          |
| (1,753) | 1:50:A:LEU:H    | 1:50:A:LEU:HD22 | 16       | 0.13          |
| (1,753) | 1:50:A:LEU:H    | 1:50:A:LEU:HD23 | 16       | 0.13          |
| (1,741) | 1:15:A:LEU:HG   | 1:16:A:CYS:HA   | 2        | 0.13          |
| (1,741) | 1:15:A:LEU:HG   | 1:16:A:CYS:HA   | 7        | 0.13          |
| (1,705) | 1:23:A:ILE:HD11 | 1:43:A:TYR:HA   | 10       | 0.13          |
| (1,705) | 1:23:A:ILE:HD12 | 1:43:A:TYR:HA   | 10       | 0.13          |
| (1,705) | 1:23:A:ILE:HD13 | 1:43:A:TYR:HA   | 10       | 0.13          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD21 | 15       | 0.13          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD22 | 15       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD23 | 15       | 0.13          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD21 | 19       | 0.13          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD22 | 19       | 0.13          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD23 | 19       | 0.13          |
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD11 | 4        | 0.13          |
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD12 | 4        | 0.13          |
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD13 | 4        | 0.13          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD11 | 4        | 0.13          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD12 | 4        | 0.13          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD13 | 4        | 0.13          |
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD11 | 4        | 0.13          |
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD12 | 4        | 0.13          |
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD13 | 4        | 0.13          |
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD11 | 5        | 0.13          |
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD12 | 5        | 0.13          |
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD13 | 5        | 0.13          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD11 | 5        | 0.13          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD12 | 5        | 0.13          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD13 | 5        | 0.13          |
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD11 | 5        | 0.13          |
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD12 | 5        | 0.13          |
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD13 | 5        | 0.13          |
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD11 | 7        | 0.13          |
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD12 | 7        | 0.13          |
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD13 | 7        | 0.13          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD11 | 7        | 0.13          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD12 | 7        | 0.13          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD13 | 7        | 0.13          |
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD11 | 7        | 0.13          |
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD12 | 7        | 0.13          |
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD13 | 7        | 0.13          |
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD11 | 11       | 0.13          |
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD12 | 11       | 0.13          |
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD13 | 11       | 0.13          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD11 | 11       | 0.13          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD12 | 11       | 0.13          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD13 | 11       | 0.13          |
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD11 | 11       | 0.13          |
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD12 | 11       | 0.13          |
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD13 | 11       | 0.13          |
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD11 | 20       | 0.13          |
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD12 | 20       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD13 | 20       | 0.13          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD11 | 20       | 0.13          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD12 | 20       | 0.13          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD13 | 20       | 0.13          |
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD11 | 20       | 0.13          |
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD12 | 20       | 0.13          |
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD13 | 20       | 0.13          |
| (1,628) | 1:34:A:LYS:H    | 1:34:A:LYS:HG2  | 15       | 0.13          |
| (1,628) | 1:34:A:LYS:H    | 1:34:A:LYS:HG2  | 18       | 0.13          |
| (1,625) | 1:8:A:ARG:HG2   | 1:59:A:PRO:HG2  | 15       | 0.13          |
| (1,625) | 1:8:A:ARG:HG3   | 1:59:A:PRO:HG2  | 15       | 0.13          |
| (1,595) | 1:16:A:CYS:HA   | 1:19:A:LEU:HB3  | 2        | 0.13          |
| (1,595) | 1:16:A:CYS:HA   | 1:19:A:LEU:HB3  | 10       | 0.13          |
| (1,595) | 1:16:A:CYS:HA   | 1:19:A:LEU:HB3  | 11       | 0.13          |
| (1,590) | 1:13:A:PRO:HB3  | 1:46:A:ALA:HB1  | 5        | 0.13          |
| (1,590) | 1:13:A:PRO:HB3  | 1:46:A:ALA:HB2  | 5        | 0.13          |
| (1,590) | 1:13:A:PRO:HB3  | 1:46:A:ALA:HB3  | 5        | 0.13          |
| (1,590) | 1:13:A:PRO:HB3  | 1:46:A:ALA:HB1  | 10       | 0.13          |
| (1,590) | 1:13:A:PRO:HB3  | 1:46:A:ALA:HB2  | 10       | 0.13          |
| (1,590) | 1:13:A:PRO:HB3  | 1:46:A:ALA:HB3  | 10       | 0.13          |
| (1,580) | 1:40:A:ARG:H    | 1:40:A:ARG:HG2  | 13       | 0.13          |
| (1,580) | 1:40:A:ARG:H    | 1:40:A:ARG:HG3  | 13       | 0.13          |
| (1,580) | 1:40:A:ARG:H    | 1:40:A:ARG:HG2  | 15       | 0.13          |
| (1,580) | 1:40:A:ARG:H    | 1:40:A:ARG:HG3  | 15       | 0.13          |
| (1,576) | 1:40:A:ARG:H    | 1:40:A:ARG:HB3  | 1        | 0.13          |
| (1,576) | 1:40:A:ARG:H    | 1:40:A:ARG:HB3  | 6        | 0.13          |
| (1,576) | 1:40:A:ARG:H    | 1:40:A:ARG:HB3  | 18       | 0.13          |
| (1,576) | 1:40:A:ARG:H    | 1:40:A:ARG:HB3  | 20       | 0.13          |
| (1,575) | 1:10:A:ARG:HA   | 1:10:A:ARG:HG3  | 1        | 0.13          |
| (1,575) | 1:10:A:ARG:HA   | 1:10:A:ARG:HG3  | 13       | 0.13          |
| (1,574) | 1:11:A:LYS:HA   | 1:11:A:LYS:HD2  | 13       | 0.13          |
| (1,574) | 1:11:A:LYS:HA   | 1:11:A:LYS:HD3  | 13       | 0.13          |
| (1,574) | 1:11:A:LYS:HA   | 1:11:A:LYS:HD2  | 18       | 0.13          |
| (1,574) | 1:11:A:LYS:HA   | 1:11:A:LYS:HD3  | 18       | 0.13          |
| (1,561) | 1:39:A:ARG:HG2  | 1:43:A:TYR:HB2  | 2        | 0.13          |
| (1,561) | 1:39:A:ARG:HG2  | 1:43:A:TYR:HB3  | 2        | 0.13          |
| (1,561) | 1:39:A:ARG:HG3  | 1:43:A:TYR:HB2  | 2        | 0.13          |
| (1,561) | 1:39:A:ARG:HG3  | 1:43:A:TYR:HB3  | 2        | 0.13          |
| (1,561) | 1:39:A:ARG:HG2  | 1:43:A:TYR:HB2  | 8        | 0.13          |
| (1,561) | 1:39:A:ARG:HG2  | 1:43:A:TYR:HB3  | 8        | 0.13          |
| (1,561) | 1:39:A:ARG:HG3  | 1:43:A:TYR:HB2  | 8        | 0.13          |
| (1,561) | 1:39:A:ARG:HG3  | 1:43:A:TYR:HB3  | 8        | 0.13          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,556) | 1:29:A:GLU:HG2 | 1:60:A:TYR:HB2 | 20       | 0.13          |
| (1,556) | 1:29:A:GLU:HG3 | 1:60:A:TYR:HB2 | 20       | 0.13          |
| (1,547) | 1:8:A:ARG:HB2  | 1:59:A:PRO:HG3 | 1        | 0.13          |
| (1,547) | 1:8:A:ARG:HB3  | 1:59:A:PRO:HG3 | 1        | 0.13          |
| (1,547) | 1:8:A:ARG:HB2  | 1:59:A:PRO:HG3 | 3        | 0.13          |
| (1,547) | 1:8:A:ARG:HB3  | 1:59:A:PRO:HG3 | 3        | 0.13          |
| (1,538) | 1:18:A:GLU:HB3 | 1:19:A:LEU:H   | 3        | 0.13          |
| (1,538) | 1:18:A:GLU:HB3 | 1:19:A:LEU:H   | 5        | 0.13          |
| (1,538) | 1:18:A:GLU:HB3 | 1:19:A:LEU:H   | 11       | 0.13          |
| (1,522) | 1:1:A:MET:HA   | 1:1:A:MET:HG2  | 2        | 0.13          |
| (1,518) | 1:40:A:ARG:H   | 1:41:A:GLU:HG2 | 5        | 0.13          |
| (1,505) | 1:41:A:GLU:HA  | 1:44:A:ASP:HB3 | 7        | 0.13          |
| (1,493) | 1:65:A:LYS:HB2 | 1:65:A:LYS:HE2 | 12       | 0.13          |
| (1,493) | 1:65:A:LYS:HB2 | 1:65:A:LYS:HE3 | 12       | 0.13          |
| (1,486) | 1:43:A:TYR:HB2 | 1:47:A:ARG:HB3 | 2        | 0.13          |
| (1,486) | 1:43:A:TYR:HB3 | 1:47:A:ARG:HB3 | 2        | 0.13          |
| (1,486) | 1:43:A:TYR:HB2 | 1:47:A:ARG:HB3 | 5        | 0.13          |
| (1,486) | 1:43:A:TYR:HB3 | 1:47:A:ARG:HB3 | 5        | 0.13          |
| (1,478) | 1:8:A:ARG:HG2  | 1:59:A:PRO:HD2 | 11       | 0.13          |
| (1,478) | 1:8:A:ARG:HG3  | 1:59:A:PRO:HD2 | 11       | 0.13          |
| (1,467) | 1:54:A:TYR:HE1 | 1:58:A:ASN:HA  | 4        | 0.13          |
| (1,467) | 1:54:A:TYR:HE2 | 1:58:A:ASN:HA  | 4        | 0.13          |
| (1,467) | 1:54:A:TYR:HE1 | 1:58:A:ASN:HA  | 6        | 0.13          |
| (1,467) | 1:54:A:TYR:HE2 | 1:58:A:ASN:HA  | 6        | 0.13          |
| (1,467) | 1:54:A:TYR:HE1 | 1:58:A:ASN:HA  | 15       | 0.13          |
| (1,467) | 1:54:A:TYR:HE2 | 1:58:A:ASN:HA  | 15       | 0.13          |
| (1,465) | 1:32:A:TYR:HE1 | 1:55:A:ARG:HG2 | 16       | 0.13          |
| (1,465) | 1:32:A:TYR:HE2 | 1:55:A:ARG:HG2 | 16       | 0.13          |
| (1,465) | 1:32:A:TYR:HE1 | 1:55:A:ARG:HG2 | 18       | 0.13          |
| (1,465) | 1:32:A:TYR:HE2 | 1:55:A:ARG:HG2 | 18       | 0.13          |
| (1,459) | 1:50:A:LEU:H   | 1:50:A:LEU:HG  | 6        | 0.13          |
| (1,459) | 1:50:A:LEU:H   | 1:50:A:LEU:HG  | 15       | 0.13          |
| (1,459) | 1:50:A:LEU:H   | 1:50:A:LEU:HG  | 20       | 0.13          |
| (1,455) | 1:54:A:TYR:HD1 | 1:59:A:PRO:HB2 | 16       | 0.13          |
| (1,455) | 1:54:A:TYR:HD2 | 1:59:A:PRO:HB2 | 16       | 0.13          |
| (1,442) | 1:76:A:TYR:HA  | 1:76:A:TYR:HE1 | 18       | 0.13          |
| (1,442) | 1:76:A:TYR:HA  | 1:76:A:TYR:HE2 | 18       | 0.13          |
| (1,439) | 1:79:A:TYR:HA  | 1:79:A:TYR:HE1 | 8        | 0.13          |
| (1,439) | 1:79:A:TYR:HA  | 1:79:A:TYR:HE2 | 8        | 0.13          |
| (1,439) | 1:79:A:TYR:HA  | 1:79:A:TYR:HE1 | 13       | 0.13          |
| (1,439) | 1:79:A:TYR:HA  | 1:79:A:TYR:HE2 | 13       | 0.13          |
| (1,418) | 1:29:A:GLU:HG2 | 1:60:A:TYR:HD1 | 18       | 0.13          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,418) | 1:29:A:GLU:HG2 | 1:60:A:TYR:HD2  | 18       | 0.13          |
| (1,418) | 1:29:A:GLU:HG3 | 1:60:A:TYR:HD1  | 18       | 0.13          |
| (1,418) | 1:29:A:GLU:HG3 | 1:60:A:TYR:HD2  | 18       | 0.13          |
| (1,418) | 1:29:A:GLU:HG2 | 1:60:A:TYR:HD1  | 20       | 0.13          |
| (1,418) | 1:29:A:GLU:HG2 | 1:60:A:TYR:HD2  | 20       | 0.13          |
| (1,418) | 1:29:A:GLU:HG3 | 1:60:A:TYR:HD1  | 20       | 0.13          |
| (1,418) | 1:29:A:GLU:HG3 | 1:60:A:TYR:HD2  | 20       | 0.13          |
| (1,410) | 1:78:A:HIS:HB3 | 1:78:A:HIS:HD2  | 19       | 0.13          |
| (1,409) | 1:78:A:HIS:HB2 | 1:78:A:HIS:HD2  | 1        | 0.13          |
| (1,409) | 1:78:A:HIS:HB2 | 1:78:A:HIS:HD2  | 5        | 0.13          |
| (1,407) | 1:38:A:LEU:HB2 | 1:41:A:GLU:H    | 17       | 0.13          |
| (1,407) | 1:38:A:LEU:HB2 | 1:41:A:GLU:H    | 19       | 0.13          |
| (1,401) | 1:32:A:TYR:HD1 | 1:55:A:ARG:HG2  | 4        | 0.13          |
| (1,401) | 1:32:A:TYR:HD2 | 1:55:A:ARG:HG2  | 4        | 0.13          |
| (1,381) | 1:78:A:HIS:HB2 | 1:79:A:TYR:HD1  | 2        | 0.13          |
| (1,381) | 1:78:A:HIS:HB2 | 1:79:A:TYR:HD2  | 2        | 0.13          |
| (1,358) | 1:24:A:HIS:HB3 | 1:24:A:HIS:HD2  | 10       | 0.13          |
| (1,358) | 1:24:A:HIS:HB3 | 1:24:A:HIS:HD2  | 20       | 0.13          |
| (1,348) | 1:66:A:CYS:HA  | 1:69:A:PHE:HZ   | 7        | 0.13          |
| (1,334) | 1:45:A:PHE:HD1 | 1:62:A:VAL:HG11 | 5        | 0.13          |
| (1,334) | 1:45:A:PHE:HD1 | 1:62:A:VAL:HG12 | 5        | 0.13          |
| (1,334) | 1:45:A:PHE:HD1 | 1:62:A:VAL:HG13 | 5        | 0.13          |
| (1,334) | 1:45:A:PHE:HD2 | 1:62:A:VAL:HG11 | 5        | 0.13          |
| (1,334) | 1:45:A:PHE:HD2 | 1:62:A:VAL:HG12 | 5        | 0.13          |
| (1,334) | 1:45:A:PHE:HD2 | 1:62:A:VAL:HG13 | 5        | 0.13          |
| (1,323) | 1:2:A:PHE:HD1  | 1:8:A:ARG:HG2   | 15       | 0.13          |
| (1,323) | 1:2:A:PHE:HD1  | 1:8:A:ARG:HG3   | 15       | 0.13          |
| (1,323) | 1:2:A:PHE:HD2  | 1:8:A:ARG:HG2   | 15       | 0.13          |
| (1,323) | 1:2:A:PHE:HD2  | 1:8:A:ARG:HG3   | 15       | 0.13          |
| (1,317) | 1:24:A:HIS:HB3 | 1:25:A:ASP:H    | 2        | 0.13          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD11 | 1        | 0.13          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD12 | 1        | 0.13          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD13 | 1        | 0.13          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD11 | 4        | 0.13          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD12 | 4        | 0.13          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD13 | 4        | 0.13          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD11 | 6        | 0.13          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD12 | 6        | 0.13          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD13 | 6        | 0.13          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD11 | 13       | 0.13          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD12 | 13       | 0.13          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD13 | 13       | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,256)  | 1:9:A:PRO:HB3  | 1:11:A:LYS:H    | 1        | 0.13          |
| (1,256)  | 1:9:A:PRO:HB3  | 1:11:A:LYS:H    | 4        | 0.13          |
| (1,256)  | 1:9:A:PRO:HB3  | 1:11:A:LYS:H    | 12       | 0.13          |
| (1,256)  | 1:9:A:PRO:HB3  | 1:11:A:LYS:H    | 16       | 0.13          |
| (1,256)  | 1:9:A:PRO:HB3  | 1:11:A:LYS:H    | 17       | 0.13          |
| (1,167)  | 1:74:A:SER:HA  | 1:75:A:GLU:H    | 15       | 0.13          |
| (1,167)  | 1:74:A:SER:HA  | 1:75:A:GLU:H    | 20       | 0.13          |
| (1,160)  | 1:35:A:GLN:H   | 1:35:A:GLN:HB3  | 11       | 0.13          |
| (1,126)  | 1:6:A:GLN:H    | 1:7:A:GLU:H     | 18       | 0.13          |
| (1,116)  | 1:44:A:ASP:H   | 1:44:A:ASP:HB3  | 1        | 0.13          |
| (1,116)  | 1:44:A:ASP:H   | 1:44:A:ASP:HB3  | 7        | 0.13          |
| (1,116)  | 1:44:A:ASP:H   | 1:44:A:ASP:HB3  | 16       | 0.13          |
| (1,116)  | 1:44:A:ASP:H   | 1:44:A:ASP:HB3  | 17       | 0.13          |
| (1,96)   | 1:35:A:GLN:HB2 | 1:36:A:GLN:H    | 9        | 0.13          |
| (1,93)   | 1:29:A:GLU:HA  | 1:36:A:GLN:H    | 9        | 0.13          |
| (1,82)   | 1:54:A:TYR:H   | 1:59:A:PRO:HA   | 1        | 0.13          |
| (1,82)   | 1:54:A:TYR:H   | 1:59:A:PRO:HA   | 7        | 0.13          |
| (1,82)   | 1:54:A:TYR:H   | 1:59:A:PRO:HA   | 18       | 0.13          |
| (1,49)   | 1:55:A:ARG:H   | 1:59:A:PRO:HA   | 8        | 0.13          |
| (1,49)   | 1:55:A:ARG:H   | 1:59:A:PRO:HA   | 11       | 0.13          |
| (1,45)   | 1:36:A:GLN:HG3 | 1:37:A:LEU:H    | 4        | 0.13          |
| (1,1240) | 1:41:A:GLU:HG2 | 1:64:A:ASP:HB2  | 9        | 0.12          |
| (1,1240) | 1:41:A:GLU:HG2 | 1:64:A:ASP:HB2  | 14       | 0.12          |
| (1,1234) | 1:10:A:ARG:HA  | 1:52:A:ILE:HD11 | 7        | 0.12          |
| (1,1234) | 1:10:A:ARG:HA  | 1:52:A:ILE:HD12 | 7        | 0.12          |
| (1,1234) | 1:10:A:ARG:HA  | 1:52:A:ILE:HD13 | 7        | 0.12          |
| (1,1234) | 1:10:A:ARG:HA  | 1:52:A:ILE:HD11 | 13       | 0.12          |
| (1,1234) | 1:10:A:ARG:HA  | 1:52:A:ILE:HD12 | 13       | 0.12          |
| (1,1234) | 1:10:A:ARG:HA  | 1:52:A:ILE:HD13 | 13       | 0.12          |
| (1,1227) | 1:2:A:PHE:HB3  | 1:54:A:TYR:HE1  | 2        | 0.12          |
| (1,1227) | 1:2:A:PHE:HB3  | 1:54:A:TYR:HE2  | 2        | 0.12          |
| (1,1227) | 1:2:A:PHE:HB3  | 1:54:A:TYR:HE1  | 14       | 0.12          |
| (1,1227) | 1:2:A:PHE:HB3  | 1:54:A:TYR:HE2  | 14       | 0.12          |
| (1,1225) | 1:2:A:PHE:HE1  | 1:54:A:TYR:HE1  | 1        | 0.12          |
| (1,1225) | 1:2:A:PHE:HE1  | 1:54:A:TYR:HE2  | 1        | 0.12          |
| (1,1225) | 1:2:A:PHE:HE2  | 1:54:A:TYR:HE1  | 1        | 0.12          |
| (1,1225) | 1:2:A:PHE:HE2  | 1:54:A:TYR:HE2  | 1        | 0.12          |
| (1,1225) | 1:2:A:PHE:HE1  | 1:54:A:TYR:HE1  | 17       | 0.12          |
| (1,1225) | 1:2:A:PHE:HE1  | 1:54:A:TYR:HE2  | 17       | 0.12          |
| (1,1225) | 1:2:A:PHE:HE2  | 1:54:A:TYR:HE1  | 17       | 0.12          |
| (1,1225) | 1:2:A:PHE:HE2  | 1:54:A:TYR:HE2  | 17       | 0.12          |
| (1,1215) | 1:3:A:GLN:HE22 | 1:4:A:ASP:HA    | 1        | 0.12          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1215) | 1:3:A:GLN:HE22  | 1:4:A:ASP:HA   | 9        | 0.12          |
| (1,1215) | 1:3:A:GLN:HE22  | 1:4:A:ASP:HA   | 13       | 0.12          |
| (1,1183) | 1:11:A:LYS:H    | 1:11:A:LYS:HB3 | 15       | 0.12          |
| (1,1177) | 1:19:A:LEU:H    | 1:19:A:LEU:HG  | 5        | 0.12          |
| (1,1170) | 1:48:A:ARG:H    | 1:48:A:ARG:HD3 | 10       | 0.12          |
| (1,1170) | 1:48:A:ARG:H    | 1:48:A:ARG:HD3 | 14       | 0.12          |
| (1,1170) | 1:48:A:ARG:H    | 1:48:A:ARG:HD3 | 17       | 0.12          |
| (1,1163) | 1:4:A:ASP:HA    | 1:6:A:GLN:H    | 20       | 0.12          |
| (1,1145) | 1:73:A:ILE:H    | 1:73:A:ILE:HB  | 20       | 0.12          |
| (1,1140) | 1:29:A:GLU:H    | 1:29:A:GLU:HB2 | 9        | 0.12          |
| (1,1140) | 1:29:A:GLU:H    | 1:29:A:GLU:HB2 | 11       | 0.12          |
| (1,1140) | 1:29:A:GLU:H    | 1:29:A:GLU:HB2 | 12       | 0.12          |
| (1,1140) | 1:29:A:GLU:H    | 1:29:A:GLU:HB2 | 14       | 0.12          |
| (1,1118) | 1:7:A:GLU:HA    | 1:8:A:ARG:H    | 5        | 0.12          |
| (1,1118) | 1:7:A:GLU:HA    | 1:8:A:ARG:H    | 14       | 0.12          |
| (1,1118) | 1:7:A:GLU:HA    | 1:8:A:ARG:H    | 16       | 0.12          |
| (1,1114) | 1:36:A:GLN:H    | 1:36:A:GLN:HG3 | 10       | 0.12          |
| (1,1108) | 1:52:A:ILE:HD11 | 1:61:A:ALA:H   | 1        | 0.12          |
| (1,1108) | 1:52:A:ILE:HD12 | 1:61:A:ALA:H   | 1        | 0.12          |
| (1,1108) | 1:52:A:ILE:HD13 | 1:61:A:ALA:H   | 1        | 0.12          |
| (1,1108) | 1:52:A:ILE:HD11 | 1:61:A:ALA:H   | 2        | 0.12          |
| (1,1108) | 1:52:A:ILE:HD12 | 1:61:A:ALA:H   | 2        | 0.12          |
| (1,1108) | 1:52:A:ILE:HD13 | 1:61:A:ALA:H   | 2        | 0.12          |
| (1,1108) | 1:52:A:ILE:HD11 | 1:61:A:ALA:H   | 4        | 0.12          |
| (1,1108) | 1:52:A:ILE:HD12 | 1:61:A:ALA:H   | 4        | 0.12          |
| (1,1108) | 1:52:A:ILE:HD13 | 1:61:A:ALA:H   | 4        | 0.12          |
| (1,1108) | 1:52:A:ILE:HD11 | 1:61:A:ALA:H   | 6        | 0.12          |
| (1,1108) | 1:52:A:ILE:HD12 | 1:61:A:ALA:H   | 6        | 0.12          |
| (1,1108) | 1:52:A:ILE:HD13 | 1:61:A:ALA:H   | 6        | 0.12          |
| (1,1108) | 1:52:A:ILE:HD11 | 1:61:A:ALA:H   | 9        | 0.12          |
| (1,1108) | 1:52:A:ILE:HD12 | 1:61:A:ALA:H   | 9        | 0.12          |
| (1,1108) | 1:52:A:ILE:HD13 | 1:61:A:ALA:H   | 9        | 0.12          |
| (1,1106) | 1:10:A:ARG:H    | 1:10:A:ARG:HB3 | 16       | 0.12          |
| (1,1072) | 1:29:A:GLU:HB2  | 1:37:A:LEU:H   | 2        | 0.12          |
| (1,1072) | 1:29:A:GLU:HB2  | 1:37:A:LEU:H   | 15       | 0.12          |
| (1,1064) | 1:26:A:ILE:HD11 | 1:28:A:LEU:HA  | 1        | 0.12          |
| (1,1064) | 1:26:A:ILE:HD12 | 1:28:A:LEU:HA  | 1        | 0.12          |
| (1,1064) | 1:26:A:ILE:HD13 | 1:28:A:LEU:HA  | 1        | 0.12          |
| (1,1064) | 1:26:A:ILE:HD11 | 1:28:A:LEU:HA  | 5        | 0.12          |
| (1,1064) | 1:26:A:ILE:HD12 | 1:28:A:LEU:HA  | 5        | 0.12          |
| (1,1064) | 1:26:A:ILE:HD13 | 1:28:A:LEU:HA  | 5        | 0.12          |
| (1,1064) | 1:26:A:ILE:HD11 | 1:28:A:LEU:HA  | 6        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1064) | 1:26:A:ILE:HD12 | 1:28:A:LEU:HA   | 6        | 0.12          |
| (1,1064) | 1:26:A:ILE:HD13 | 1:28:A:LEU:HA   | 6        | 0.12          |
| (1,1064) | 1:26:A:ILE:HD11 | 1:28:A:LEU:HA   | 17       | 0.12          |
| (1,1064) | 1:26:A:ILE:HD12 | 1:28:A:LEU:HA   | 17       | 0.12          |
| (1,1064) | 1:26:A:ILE:HD13 | 1:28:A:LEU:HA   | 17       | 0.12          |
| (1,1064) | 1:26:A:ILE:HD11 | 1:28:A:LEU:HA   | 19       | 0.12          |
| (1,1064) | 1:26:A:ILE:HD12 | 1:28:A:LEU:HA   | 19       | 0.12          |
| (1,1064) | 1:26:A:ILE:HD13 | 1:28:A:LEU:HA   | 19       | 0.12          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB1  | 16       | 0.12          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB2  | 16       | 0.12          |
| (1,1042) | 1:28:A:LEU:HA   | 1:61:A:ALA:HB3  | 16       | 0.12          |
| (1,1035) | 1:17:A:THR:HG21 | 1:18:A:GLU:HG3  | 2        | 0.12          |
| (1,1035) | 1:17:A:THR:HG22 | 1:18:A:GLU:HG3  | 2        | 0.12          |
| (1,1035) | 1:17:A:THR:HG23 | 1:18:A:GLU:HG3  | 2        | 0.12          |
| (1,1035) | 1:17:A:THR:HG21 | 1:18:A:GLU:HG3  | 4        | 0.12          |
| (1,1035) | 1:17:A:THR:HG22 | 1:18:A:GLU:HG3  | 4        | 0.12          |
| (1,1035) | 1:17:A:THR:HG23 | 1:18:A:GLU:HG3  | 4        | 0.12          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG11 | 11       | 0.12          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG12 | 11       | 0.12          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG13 | 11       | 0.12          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG11 | 14       | 0.12          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG12 | 14       | 0.12          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG13 | 14       | 0.12          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG11 | 16       | 0.12          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG12 | 16       | 0.12          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG13 | 16       | 0.12          |
| (1,1014) | 1:11:A:LYS:HG3  | 1:14:A:GLN:HE21 | 11       | 0.12          |
| (1,984)  | 1:26:A:ILE:HG13 | 1:28:A:LEU:HA   | 1        | 0.12          |
| (1,984)  | 1:26:A:ILE:HG13 | 1:28:A:LEU:HA   | 3        | 0.12          |
| (1,984)  | 1:26:A:ILE:HG13 | 1:28:A:LEU:HA   | 12       | 0.12          |
| (1,984)  | 1:26:A:ILE:HG13 | 1:28:A:LEU:HA   | 17       | 0.12          |
| (1,984)  | 1:26:A:ILE:HG13 | 1:28:A:LEU:HA   | 20       | 0.12          |
| (1,964)  | 1:53:A:VAL:HG21 | 1:62:A:VAL:HB   | 11       | 0.12          |
| (1,964)  | 1:53:A:VAL:HG22 | 1:62:A:VAL:HB   | 11       | 0.12          |
| (1,964)  | 1:53:A:VAL:HG23 | 1:62:A:VAL:HB   | 11       | 0.12          |
| (1,964)  | 1:53:A:VAL:HG21 | 1:62:A:VAL:HB   | 20       | 0.12          |
| (1,964)  | 1:53:A:VAL:HG22 | 1:62:A:VAL:HB   | 20       | 0.12          |
| (1,964)  | 1:53:A:VAL:HG23 | 1:62:A:VAL:HB   | 20       | 0.12          |
| (1,958)  | 1:29:A:GLU:HA   | 1:29:A:GLU:HG2  | 7        | 0.12          |
| (1,958)  | 1:29:A:GLU:HA   | 1:29:A:GLU:HG3  | 7        | 0.12          |
| (1,932)  | 1:10:A:ARG:HA   | 1:10:A:ARG:HD2  | 2        | 0.12          |
| (1,932)  | 1:10:A:ARG:HA   | 1:10:A:ARG:HD3  | 2        | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,924) | 1:9:A:PRO:HD2   | 1:15:A:LEU:HB3  | 11       | 0.12          |
| (1,924) | 1:9:A:PRO:HD2   | 1:15:A:LEU:HB3  | 14       | 0.12          |
| (1,924) | 1:9:A:PRO:HD2   | 1:15:A:LEU:HB3  | 20       | 0.12          |
| (1,907) | 1:77:A:ARG:HA   | 1:77:A:ARG:HG2  | 9        | 0.12          |
| (1,907) | 1:77:A:ARG:HA   | 1:77:A:ARG:HG3  | 9        | 0.12          |
| (1,905) | 1:77:A:ARG:HA   | 1:77:A:ARG:HD2  | 4        | 0.12          |
| (1,905) | 1:77:A:ARG:HA   | 1:77:A:ARG:HD3  | 4        | 0.12          |
| (1,872) | 1:73:A:ILE:HB   | 1:74:A:SER:HA   | 12       | 0.12          |
| (1,864) | 1:69:A:PHE:HA   | 1:69:A:PHE:HB2  | 1        | 0.12          |
| (1,864) | 1:69:A:PHE:HA   | 1:69:A:PHE:HB2  | 5        | 0.12          |
| (1,864) | 1:69:A:PHE:HA   | 1:69:A:PHE:HB2  | 6        | 0.12          |
| (1,864) | 1:69:A:PHE:HA   | 1:69:A:PHE:HB2  | 8        | 0.12          |
| (1,864) | 1:69:A:PHE:HA   | 1:69:A:PHE:HB2  | 13       | 0.12          |
| (1,864) | 1:69:A:PHE:HA   | 1:69:A:PHE:HB2  | 19       | 0.12          |
| (1,854) | 1:73:A:ILE:HA   | 1:73:A:ILE:HG12 | 20       | 0.12          |
| (1,850) | 1:23:A:ILE:HA   | 1:23:A:ILE:HG13 | 6        | 0.12          |
| (1,850) | 1:23:A:ILE:HA   | 1:23:A:ILE:HG13 | 11       | 0.12          |
| (1,745) | 1:50:A:LEU:HA   | 1:50:A:LEU:HD11 | 16       | 0.12          |
| (1,745) | 1:50:A:LEU:HA   | 1:50:A:LEU:HD12 | 16       | 0.12          |
| (1,745) | 1:50:A:LEU:HA   | 1:50:A:LEU:HD13 | 16       | 0.12          |
| (1,741) | 1:15:A:LEU:HG   | 1:16:A:CYS:HA   | 8        | 0.12          |
| (1,741) | 1:15:A:LEU:HG   | 1:16:A:CYS:HA   | 15       | 0.12          |
| (1,706) | 1:23:A:ILE:HA   | 1:23:A:ILE:HD11 | 10       | 0.12          |
| (1,706) | 1:23:A:ILE:HA   | 1:23:A:ILE:HD12 | 10       | 0.12          |
| (1,706) | 1:23:A:ILE:HA   | 1:23:A:ILE:HD13 | 10       | 0.12          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD21 | 14       | 0.12          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD22 | 14       | 0.12          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD23 | 14       | 0.12          |
| (1,691) | 1:18:A:GLU:HG3  | 1:19:A:LEU:HD11 | 1        | 0.12          |
| (1,691) | 1:18:A:GLU:HG3  | 1:19:A:LEU:HD12 | 1        | 0.12          |
| (1,691) | 1:18:A:GLU:HG3  | 1:19:A:LEU:HD13 | 1        | 0.12          |
| (1,689) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD11 | 7        | 0.12          |
| (1,689) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD12 | 7        | 0.12          |
| (1,689) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD13 | 7        | 0.12          |
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD11 | 3        | 0.12          |
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD12 | 3        | 0.12          |
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD13 | 3        | 0.12          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD11 | 3        | 0.12          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD12 | 3        | 0.12          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD13 | 3        | 0.12          |
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD11 | 3        | 0.12          |
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD12 | 3        | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD13 | 3        | 0.12          |
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD11 | 15       | 0.12          |
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD12 | 15       | 0.12          |
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD13 | 15       | 0.12          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD11 | 15       | 0.12          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD12 | 15       | 0.12          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD13 | 15       | 0.12          |
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD11 | 15       | 0.12          |
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD12 | 15       | 0.12          |
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD13 | 15       | 0.12          |
| (1,664) | 1:12:A:LEU:HD11 | 1:15:A:LEU:HB2  | 6        | 0.12          |
| (1,664) | 1:12:A:LEU:HD12 | 1:15:A:LEU:HB2  | 6        | 0.12          |
| (1,664) | 1:12:A:LEU:HD13 | 1:15:A:LEU:HB2  | 6        | 0.12          |
| (1,660) | 1:12:A:LEU:HD11 | 1:61:A:ALA:HA   | 7        | 0.12          |
| (1,660) | 1:12:A:LEU:HD12 | 1:61:A:ALA:HA   | 7        | 0.12          |
| (1,660) | 1:12:A:LEU:HD13 | 1:61:A:ALA:HA   | 7        | 0.12          |
| (1,625) | 1:8:A:ARG:HG2   | 1:59:A:PRO:HG2  | 7        | 0.12          |
| (1,625) | 1:8:A:ARG:HG3   | 1:59:A:PRO:HG2  | 7        | 0.12          |
| (1,625) | 1:8:A:ARG:HG2   | 1:59:A:PRO:HG2  | 8        | 0.12          |
| (1,625) | 1:8:A:ARG:HG3   | 1:59:A:PRO:HG2  | 8        | 0.12          |
| (1,625) | 1:8:A:ARG:HG2   | 1:59:A:PRO:HG2  | 9        | 0.12          |
| (1,625) | 1:8:A:ARG:HG3   | 1:59:A:PRO:HG2  | 9        | 0.12          |
| (1,606) | 1:34:A:LYS:HA   | 1:34:A:LYS:HD3  | 17       | 0.12          |
| (1,595) | 1:16:A:CYS:HA   | 1:19:A:LEU:HB3  | 12       | 0.12          |
| (1,595) | 1:16:A:CYS:HA   | 1:19:A:LEU:HB3  | 18       | 0.12          |
| (1,590) | 1:13:A:PRO:HB3  | 1:46:A:ALA:HB1  | 6        | 0.12          |
| (1,590) | 1:13:A:PRO:HB3  | 1:46:A:ALA:HB2  | 6        | 0.12          |
| (1,590) | 1:13:A:PRO:HB3  | 1:46:A:ALA:HB3  | 6        | 0.12          |
| (1,584) | 1:22:A:THR:HB   | 1:23:A:ILE:HB   | 9        | 0.12          |
| (1,580) | 1:40:A:ARG:H    | 1:40:A:ARG:HG2  | 9        | 0.12          |
| (1,580) | 1:40:A:ARG:H    | 1:40:A:ARG:HG3  | 9        | 0.12          |
| (1,578) | 1:67:A:LEU:H    | 1:67:A:LEU:HG   | 3        | 0.12          |
| (1,576) | 1:40:A:ARG:H    | 1:40:A:ARG:HB3  | 12       | 0.12          |
| (1,574) | 1:11:A:LYS:HA   | 1:11:A:LYS:HD2  | 14       | 0.12          |
| (1,574) | 1:11:A:LYS:HA   | 1:11:A:LYS:HD3  | 14       | 0.12          |
| (1,574) | 1:11:A:LYS:HA   | 1:11:A:LYS:HD2  | 16       | 0.12          |
| (1,574) | 1:11:A:LYS:HA   | 1:11:A:LYS:HD3  | 16       | 0.12          |
| (1,561) | 1:39:A:ARG:HG2  | 1:43:A:TYR:HB2  | 7        | 0.12          |
| (1,561) | 1:39:A:ARG:HG2  | 1:43:A:TYR:HB3  | 7        | 0.12          |
| (1,561) | 1:39:A:ARG:HG3  | 1:43:A:TYR:HB2  | 7        | 0.12          |
| (1,561) | 1:39:A:ARG:HG3  | 1:43:A:TYR:HB3  | 7        | 0.12          |
| (1,556) | 1:29:A:GLU:HG2  | 1:60:A:TYR:HB2  | 3        | 0.12          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,556) | 1:29:A:GLU:HG3 | 1:60:A:TYR:HB2 | 3        | 0.12          |
| (1,556) | 1:29:A:GLU:HG2 | 1:60:A:TYR:HB2 | 9        | 0.12          |
| (1,556) | 1:29:A:GLU:HG3 | 1:60:A:TYR:HB2 | 9        | 0.12          |
| (1,556) | 1:29:A:GLU:HG2 | 1:60:A:TYR:HB2 | 14       | 0.12          |
| (1,556) | 1:29:A:GLU:HG3 | 1:60:A:TYR:HB2 | 14       | 0.12          |
| (1,547) | 1:8:A:ARG:HB2  | 1:59:A:PRO:HG3 | 15       | 0.12          |
| (1,547) | 1:8:A:ARG:HB3  | 1:59:A:PRO:HG3 | 15       | 0.12          |
| (1,547) | 1:8:A:ARG:HB2  | 1:59:A:PRO:HG3 | 19       | 0.12          |
| (1,547) | 1:8:A:ARG:HB3  | 1:59:A:PRO:HG3 | 19       | 0.12          |
| (1,538) | 1:18:A:GLU:HB3 | 1:19:A:LEU:H   | 7        | 0.12          |
| (1,538) | 1:18:A:GLU:HB3 | 1:19:A:LEU:H   | 8        | 0.12          |
| (1,538) | 1:18:A:GLU:HB3 | 1:19:A:LEU:H   | 19       | 0.12          |
| (1,522) | 1:1:A:MET:HA   | 1:1:A:MET:HG2  | 14       | 0.12          |
| (1,518) | 1:40:A:ARG:H   | 1:41:A:GLU:HG2 | 17       | 0.12          |
| (1,518) | 1:40:A:ARG:H   | 1:41:A:GLU:HG2 | 19       | 0.12          |
| (1,518) | 1:40:A:ARG:H   | 1:41:A:GLU:HG2 | 20       | 0.12          |
| (1,505) | 1:41:A:GLU:HA  | 1:44:A:ASP:HB3 | 3        | 0.12          |
| (1,486) | 1:43:A:TYR:HB2 | 1:47:A:ARG:HB3 | 13       | 0.12          |
| (1,486) | 1:43:A:TYR:HB3 | 1:47:A:ARG:HB3 | 13       | 0.12          |
| (1,483) | 1:43:A:TYR:HB2 | 1:47:A:ARG:HB2 | 3        | 0.12          |
| (1,483) | 1:43:A:TYR:HB3 | 1:47:A:ARG:HB2 | 3        | 0.12          |
| (1,478) | 1:8:A:ARG:HG2  | 1:59:A:PRO:HD2 | 2        | 0.12          |
| (1,478) | 1:8:A:ARG:HG3  | 1:59:A:PRO:HD2 | 2        | 0.12          |
| (1,478) | 1:8:A:ARG:HG2  | 1:59:A:PRO:HD2 | 6        | 0.12          |
| (1,478) | 1:8:A:ARG:HG3  | 1:59:A:PRO:HD2 | 6        | 0.12          |
| (1,478) | 1:8:A:ARG:HG2  | 1:59:A:PRO:HD2 | 13       | 0.12          |
| (1,478) | 1:8:A:ARG:HG3  | 1:59:A:PRO:HD2 | 13       | 0.12          |
| (1,477) | 1:77:A:ARG:H   | 1:78:A:HIS:HA  | 7        | 0.12          |
| (1,467) | 1:54:A:TYR:HE1 | 1:58:A:ASN:HA  | 1        | 0.12          |
| (1,467) | 1:54:A:TYR:HE2 | 1:58:A:ASN:HA  | 1        | 0.12          |
| (1,467) | 1:54:A:TYR:HE1 | 1:58:A:ASN:HA  | 14       | 0.12          |
| (1,467) | 1:54:A:TYR:HE2 | 1:58:A:ASN:HA  | 14       | 0.12          |
| (1,465) | 1:32:A:TYR:HE1 | 1:55:A:ARG:HG2 | 5        | 0.12          |
| (1,465) | 1:32:A:TYR:HE2 | 1:55:A:ARG:HG2 | 5        | 0.12          |
| (1,465) | 1:32:A:TYR:HE1 | 1:55:A:ARG:HG2 | 8        | 0.12          |
| (1,465) | 1:32:A:TYR:HE2 | 1:55:A:ARG:HG2 | 8        | 0.12          |
| (1,465) | 1:32:A:TYR:HE1 | 1:55:A:ARG:HG2 | 11       | 0.12          |
| (1,465) | 1:32:A:TYR:HE2 | 1:55:A:ARG:HG2 | 11       | 0.12          |
| (1,464) | 1:32:A:TYR:HA  | 1:32:A:TYR:HE1 | 2        | 0.12          |
| (1,464) | 1:32:A:TYR:HA  | 1:32:A:TYR:HE2 | 2        | 0.12          |
| (1,464) | 1:32:A:TYR:HA  | 1:32:A:TYR:HE1 | 4        | 0.12          |
| (1,464) | 1:32:A:TYR:HA  | 1:32:A:TYR:HE2 | 4        | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,464) | 1:32:A:TYR:HA   | 1:32:A:TYR:HE1  | 8        | 0.12          |
| (1,464) | 1:32:A:TYR:HA   | 1:32:A:TYR:HE2  | 8        | 0.12          |
| (1,464) | 1:32:A:TYR:HA   | 1:32:A:TYR:HE1  | 12       | 0.12          |
| (1,464) | 1:32:A:TYR:HA   | 1:32:A:TYR:HE2  | 12       | 0.12          |
| (1,464) | 1:32:A:TYR:HA   | 1:32:A:TYR:HE1  | 20       | 0.12          |
| (1,464) | 1:32:A:TYR:HA   | 1:32:A:TYR:HE2  | 20       | 0.12          |
| (1,459) | 1:50:A:LEU:H    | 1:50:A:LEU:HG   | 8        | 0.12          |
| (1,459) | 1:50:A:LEU:H    | 1:50:A:LEU:HG   | 11       | 0.12          |
| (1,459) | 1:50:A:LEU:H    | 1:50:A:LEU:HG   | 18       | 0.12          |
| (1,443) | 1:76:A:TYR:HE1  | 1:78:A:HIS:HB3  | 3        | 0.12          |
| (1,443) | 1:76:A:TYR:HE2  | 1:78:A:HIS:HB3  | 3        | 0.12          |
| (1,439) | 1:79:A:TYR:HA   | 1:79:A:TYR:HE1  | 16       | 0.12          |
| (1,439) | 1:79:A:TYR:HA   | 1:79:A:TYR:HE2  | 16       | 0.12          |
| (1,430) | 1:3:A:GLN:HA    | 1:3:A:GLN:HE22  | 13       | 0.12          |
| (1,430) | 1:3:A:GLN:HA    | 1:3:A:GLN:HE22  | 15       | 0.12          |
| (1,409) | 1:78:A:HIS:HB2  | 1:78:A:HIS:HD2  | 3        | 0.12          |
| (1,409) | 1:78:A:HIS:HB2  | 1:78:A:HIS:HD2  | 7        | 0.12          |
| (1,409) | 1:78:A:HIS:HB2  | 1:78:A:HIS:HD2  | 13       | 0.12          |
| (1,401) | 1:32:A:TYR:HD1  | 1:55:A:ARG:HG2  | 1        | 0.12          |
| (1,401) | 1:32:A:TYR:HD2  | 1:55:A:ARG:HG2  | 1        | 0.12          |
| (1,401) | 1:32:A:TYR:HD1  | 1:55:A:ARG:HG2  | 2        | 0.12          |
| (1,401) | 1:32:A:TYR:HD2  | 1:55:A:ARG:HG2  | 2        | 0.12          |
| (1,401) | 1:32:A:TYR:HD1  | 1:55:A:ARG:HG2  | 6        | 0.12          |
| (1,401) | 1:32:A:TYR:HD2  | 1:55:A:ARG:HG2  | 6        | 0.12          |
| (1,401) | 1:32:A:TYR:HD1  | 1:55:A:ARG:HG2  | 17       | 0.12          |
| (1,401) | 1:32:A:TYR:HD2  | 1:55:A:ARG:HG2  | 17       | 0.12          |
| (1,387) | 1:58:A:ASN:HD22 | 1:60:A:TYR:HE1  | 20       | 0.12          |
| (1,387) | 1:58:A:ASN:HD22 | 1:60:A:TYR:HE2  | 20       | 0.12          |
| (1,381) | 1:78:A:HIS:HB2  | 1:79:A:TYR:HD1  | 7        | 0.12          |
| (1,381) | 1:78:A:HIS:HB2  | 1:79:A:TYR:HD2  | 7        | 0.12          |
| (1,358) | 1:24:A:HIS:HB3  | 1:24:A:HIS:HD2  | 9        | 0.12          |
| (1,358) | 1:24:A:HIS:HB3  | 1:24:A:HIS:HD2  | 17       | 0.12          |
| (1,358) | 1:24:A:HIS:HB3  | 1:24:A:HIS:HD2  | 19       | 0.12          |
| (1,334) | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG11 | 4        | 0.12          |
| (1,334) | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG12 | 4        | 0.12          |
| (1,334) | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG13 | 4        | 0.12          |
| (1,334) | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG11 | 4        | 0.12          |
| (1,334) | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG12 | 4        | 0.12          |
| (1,334) | 1:45:A:PHE:HD2  | 1:62:A:VAL:HG13 | 4        | 0.12          |
| (1,334) | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG11 | 18       | 0.12          |
| (1,334) | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG12 | 18       | 0.12          |
| (1,334) | 1:45:A:PHE:HD1  | 1:62:A:VAL:HG13 | 18       | 0.12          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,334)  | 1:45:A:PHE:HD2 | 1:62:A:VAL:HG11 | 18       | 0.12          |
| (1,334)  | 1:45:A:PHE:HD2 | 1:62:A:VAL:HG12 | 18       | 0.12          |
| (1,334)  | 1:45:A:PHE:HD2 | 1:62:A:VAL:HG13 | 18       | 0.12          |
| (1,321)  | 1:2:A:PHE:HD1  | 1:19:A:LEU:HG   | 11       | 0.12          |
| (1,321)  | 1:2:A:PHE:HD2  | 1:19:A:LEU:HG   | 11       | 0.12          |
| (1,317)  | 1:24:A:HIS:HB3 | 1:25:A:ASP:H    | 16       | 0.12          |
| (1,306)  | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD11 | 20       | 0.12          |
| (1,306)  | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD12 | 20       | 0.12          |
| (1,306)  | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD13 | 20       | 0.12          |
| (1,256)  | 1:9:A:PRO:HB3  | 1:11:A:LYS:H    | 5        | 0.12          |
| (1,256)  | 1:9:A:PRO:HB3  | 1:11:A:LYS:H    | 7        | 0.12          |
| (1,256)  | 1:9:A:PRO:HB3  | 1:11:A:LYS:H    | 8        | 0.12          |
| (1,256)  | 1:9:A:PRO:HB3  | 1:11:A:LYS:H    | 9        | 0.12          |
| (1,235)  | 1:30:A:CYS:HB2 | 1:34:A:LYS:H    | 10       | 0.12          |
| (1,216)  | 1:46:A:ALA:HB1 | 1:48:A:ARG:H    | 13       | 0.12          |
| (1,216)  | 1:46:A:ALA:HB2 | 1:48:A:ARG:H    | 13       | 0.12          |
| (1,216)  | 1:46:A:ALA:HB3 | 1:48:A:ARG:H    | 13       | 0.12          |
| (1,207)  | 1:76:A:TYR:H   | 1:76:A:TYR:HD1  | 2        | 0.12          |
| (1,207)  | 1:76:A:TYR:H   | 1:76:A:TYR:HD2  | 2        | 0.12          |
| (1,167)  | 1:74:A:SER:HA  | 1:75:A:GLU:H    | 4        | 0.12          |
| (1,160)  | 1:35:A:GLN:H   | 1:35:A:GLN:HB3  | 9        | 0.12          |
| (1,116)  | 1:44:A:ASP:H   | 1:44:A:ASP:HB3  | 3        | 0.12          |
| (1,116)  | 1:44:A:ASP:H   | 1:44:A:ASP:HB3  | 6        | 0.12          |
| (1,116)  | 1:44:A:ASP:H   | 1:44:A:ASP:HB3  | 12       | 0.12          |
| (1,96)   | 1:35:A:GLN:HB2 | 1:36:A:GLN:H    | 14       | 0.12          |
| (1,93)   | 1:29:A:GLU:HA  | 1:36:A:GLN:H    | 16       | 0.12          |
| (1,82)   | 1:54:A:TYR:H   | 1:59:A:PRO:HA   | 4        | 0.12          |
| (1,82)   | 1:54:A:TYR:H   | 1:59:A:PRO:HA   | 8        | 0.12          |
| (1,72)   | 1:10:A:ARG:H   | 1:11:A:LYS:HG3  | 15       | 0.12          |
| (1,45)   | 1:36:A:GLN:HG3 | 1:37:A:LEU:H    | 9        | 0.12          |
| (1,1232) | 1:24:A:HIS:HA  | 1:43:A:TYR:HE1  | 18       | 0.11          |
| (1,1232) | 1:24:A:HIS:HA  | 1:43:A:TYR:HE2  | 18       | 0.11          |
| (1,1231) | 1:54:A:TYR:HA  | 1:60:A:TYR:HE1  | 11       | 0.11          |
| (1,1231) | 1:54:A:TYR:HA  | 1:60:A:TYR:HE2  | 11       | 0.11          |
| (1,1228) | 1:9:A:PRO:HG2  | 1:54:A:TYR:HE1  | 7        | 0.11          |
| (1,1228) | 1:9:A:PRO:HG2  | 1:54:A:TYR:HE2  | 7        | 0.11          |
| (1,1228) | 1:9:A:PRO:HG3  | 1:54:A:TYR:HE1  | 7        | 0.11          |
| (1,1228) | 1:9:A:PRO:HG3  | 1:54:A:TYR:HE2  | 7        | 0.11          |
| (1,1228) | 1:9:A:PRO:HG2  | 1:54:A:TYR:HE1  | 8        | 0.11          |
| (1,1228) | 1:9:A:PRO:HG2  | 1:54:A:TYR:HE2  | 8        | 0.11          |
| (1,1228) | 1:9:A:PRO:HG3  | 1:54:A:TYR:HE1  | 8        | 0.11          |
| (1,1228) | 1:9:A:PRO:HG3  | 1:54:A:TYR:HE2  | 8        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1225) | 1:2:A:PHE:HE1   | 1:54:A:TYR:HE1  | 3        | 0.11          |
| (1,1225) | 1:2:A:PHE:HE1   | 1:54:A:TYR:HE2  | 3        | 0.11          |
| (1,1225) | 1:2:A:PHE:HE2   | 1:54:A:TYR:HE1  | 3        | 0.11          |
| (1,1225) | 1:2:A:PHE:HE2   | 1:54:A:TYR:HE2  | 3        | 0.11          |
| (1,1225) | 1:2:A:PHE:HE1   | 1:54:A:TYR:HE1  | 20       | 0.11          |
| (1,1225) | 1:2:A:PHE:HE1   | 1:54:A:TYR:HE2  | 20       | 0.11          |
| (1,1225) | 1:2:A:PHE:HE2   | 1:54:A:TYR:HE1  | 20       | 0.11          |
| (1,1225) | 1:2:A:PHE:HE2   | 1:54:A:TYR:HE2  | 20       | 0.11          |
| (1,1218) | 1:3:A:GLN:HE21  | 1:4:A:ASP:HA    | 2        | 0.11          |
| (1,1215) | 1:3:A:GLN:HE22  | 1:4:A:ASP:HA    | 3        | 0.11          |
| (1,1203) | 1:35:A:GLN:HA   | 1:35:A:GLN:HE22 | 2        | 0.11          |
| (1,1203) | 1:35:A:GLN:HA   | 1:35:A:GLN:HE22 | 20       | 0.11          |
| (1,1183) | 1:11:A:LYS:H    | 1:11:A:LYS:HB3  | 19       | 0.11          |
| (1,1177) | 1:19:A:LEU:H    | 1:19:A:LEU:HG   | 19       | 0.11          |
| (1,1170) | 1:48:A:ARG:H    | 1:48:A:ARG:HD3  | 3        | 0.11          |
| (1,1170) | 1:48:A:ARG:H    | 1:48:A:ARG:HD3  | 5        | 0.11          |
| (1,1170) | 1:48:A:ARG:H    | 1:48:A:ARG:HD3  | 6        | 0.11          |
| (1,1170) | 1:48:A:ARG:H    | 1:48:A:ARG:HD3  | 8        | 0.11          |
| (1,1170) | 1:48:A:ARG:H    | 1:48:A:ARG:HD3  | 9        | 0.11          |
| (1,1170) | 1:48:A:ARG:H    | 1:48:A:ARG:HD3  | 16       | 0.11          |
| (1,1152) | 1:70:A:TYR:H    | 1:70:A:TYR:HB3  | 7        | 0.11          |
| (1,1142) | 1:69:A:PHE:H    | 1:69:A:PHE:HB3  | 7        | 0.11          |
| (1,1142) | 1:69:A:PHE:H    | 1:69:A:PHE:HB3  | 12       | 0.11          |
| (1,1142) | 1:69:A:PHE:H    | 1:69:A:PHE:HB3  | 20       | 0.11          |
| (1,1140) | 1:29:A:GLU:H    | 1:29:A:GLU:HB2  | 1        | 0.11          |
| (1,1140) | 1:29:A:GLU:H    | 1:29:A:GLU:HB2  | 2        | 0.11          |
| (1,1140) | 1:29:A:GLU:H    | 1:29:A:GLU:HB2  | 8        | 0.11          |
| (1,1118) | 1:7:A:GLU:HA    | 1:8:A:ARG:H     | 11       | 0.11          |
| (1,1117) | 1:2:A:PHE:HB2   | 1:3:A:GLN:H     | 9        | 0.11          |
| (1,1114) | 1:36:A:GLN:H    | 1:36:A:GLN:HG3  | 1        | 0.11          |
| (1,1108) | 1:52:A:ILE:HD11 | 1:61:A:ALA:H    | 7        | 0.11          |
| (1,1108) | 1:52:A:ILE:HD12 | 1:61:A:ALA:H    | 7        | 0.11          |
| (1,1108) | 1:52:A:ILE:HD13 | 1:61:A:ALA:H    | 7        | 0.11          |
| (1,1108) | 1:52:A:ILE:HD11 | 1:61:A:ALA:H    | 14       | 0.11          |
| (1,1108) | 1:52:A:ILE:HD12 | 1:61:A:ALA:H    | 14       | 0.11          |
| (1,1108) | 1:52:A:ILE:HD13 | 1:61:A:ALA:H    | 14       | 0.11          |
| (1,1108) | 1:52:A:ILE:HD11 | 1:61:A:ALA:H    | 20       | 0.11          |
| (1,1108) | 1:52:A:ILE:HD12 | 1:61:A:ALA:H    | 20       | 0.11          |
| (1,1108) | 1:52:A:ILE:HD13 | 1:61:A:ALA:H    | 20       | 0.11          |
| (1,1106) | 1:10:A:ARG:H    | 1:10:A:ARG:HB3  | 6        | 0.11          |
| (1,1072) | 1:29:A:GLU:HB2  | 1:37:A:LEU:H    | 1        | 0.11          |
| (1,1072) | 1:29:A:GLU:HB2  | 1:37:A:LEU:H    | 11       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1064) | 1:26:A:ILE:HD11 | 1:28:A:LEU:HA   | 10       | 0.11          |
| (1,1064) | 1:26:A:ILE:HD12 | 1:28:A:LEU:HA   | 10       | 0.11          |
| (1,1064) | 1:26:A:ILE:HD13 | 1:28:A:LEU:HA   | 10       | 0.11          |
| (1,1064) | 1:26:A:ILE:HD11 | 1:28:A:LEU:HA   | 13       | 0.11          |
| (1,1064) | 1:26:A:ILE:HD12 | 1:28:A:LEU:HA   | 13       | 0.11          |
| (1,1064) | 1:26:A:ILE:HD13 | 1:28:A:LEU:HA   | 13       | 0.11          |
| (1,1064) | 1:26:A:ILE:HD11 | 1:28:A:LEU:HA   | 14       | 0.11          |
| (1,1064) | 1:26:A:ILE:HD12 | 1:28:A:LEU:HA   | 14       | 0.11          |
| (1,1064) | 1:26:A:ILE:HD13 | 1:28:A:LEU:HA   | 14       | 0.11          |
| (1,1064) | 1:26:A:ILE:HD11 | 1:28:A:LEU:HA   | 16       | 0.11          |
| (1,1064) | 1:26:A:ILE:HD12 | 1:28:A:LEU:HA   | 16       | 0.11          |
| (1,1064) | 1:26:A:ILE:HD13 | 1:28:A:LEU:HA   | 16       | 0.11          |
| (1,1064) | 1:26:A:ILE:HD11 | 1:28:A:LEU:HA   | 18       | 0.11          |
| (1,1064) | 1:26:A:ILE:HD12 | 1:28:A:LEU:HA   | 18       | 0.11          |
| (1,1064) | 1:26:A:ILE:HD13 | 1:28:A:LEU:HA   | 18       | 0.11          |
| (1,1057) | 1:1:A:MET:HE1   | 1:2:A:PHE:HA    | 5        | 0.11          |
| (1,1057) | 1:1:A:MET:HE2   | 1:2:A:PHE:HA    | 5        | 0.11          |
| (1,1057) | 1:1:A:MET:HE3   | 1:2:A:PHE:HA    | 5        | 0.11          |
| (1,1035) | 1:17:A:THR:HG21 | 1:18:A:GLU:HG3  | 14       | 0.11          |
| (1,1035) | 1:17:A:THR:HG22 | 1:18:A:GLU:HG3  | 14       | 0.11          |
| (1,1035) | 1:17:A:THR:HG23 | 1:18:A:GLU:HG3  | 14       | 0.11          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG11 | 6        | 0.11          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG12 | 6        | 0.11          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG13 | 6        | 0.11          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG11 | 8        | 0.11          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG12 | 8        | 0.11          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG13 | 8        | 0.11          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG11 | 19       | 0.11          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG12 | 19       | 0.11          |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG13 | 19       | 0.11          |
| (1,997)  | 1:38:A:LEU:H    | 1:38:A:LEU:HG   | 1        | 0.11          |
| (1,984)  | 1:26:A:ILE:HG13 | 1:28:A:LEU:HA   | 2        | 0.11          |
| (1,984)  | 1:26:A:ILE:HG13 | 1:28:A:LEU:HA   | 5        | 0.11          |
| (1,984)  | 1:26:A:ILE:HG13 | 1:28:A:LEU:HA   | 6        | 0.11          |
| (1,964)  | 1:53:A:VAL:HG21 | 1:62:A:VAL:HB   | 6        | 0.11          |
| (1,964)  | 1:53:A:VAL:HG22 | 1:62:A:VAL:HB   | 6        | 0.11          |
| (1,964)  | 1:53:A:VAL:HG23 | 1:62:A:VAL:HB   | 6        | 0.11          |
| (1,964)  | 1:53:A:VAL:HG21 | 1:62:A:VAL:HB   | 17       | 0.11          |
| (1,964)  | 1:53:A:VAL:HG22 | 1:62:A:VAL:HB   | 17       | 0.11          |
| (1,964)  | 1:53:A:VAL:HG23 | 1:62:A:VAL:HB   | 17       | 0.11          |
| (1,962)  | 1:7:A:GLU:HA    | 1:7:A:GLU:HG3   | 8        | 0.11          |
| (1,962)  | 1:7:A:GLU:HA    | 1:7:A:GLU:HG3   | 13       | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,932) | 1:10:A:ARG:HA   | 1:10:A:ARG:HD2  | 12       | 0.11          |
| (1,932) | 1:10:A:ARG:HA   | 1:10:A:ARG:HD3  | 12       | 0.11          |
| (1,888) | 1:44:A:ASP:HA   | 1:47:A:ARG:H    | 8        | 0.11          |
| (1,888) | 1:44:A:ASP:HA   | 1:47:A:ARG:H    | 11       | 0.11          |
| (1,867) | 1:15:A:LEU:HD11 | 1:18:A:GLU:HA   | 5        | 0.11          |
| (1,867) | 1:15:A:LEU:HD12 | 1:18:A:GLU:HA   | 5        | 0.11          |
| (1,867) | 1:15:A:LEU:HD13 | 1:18:A:GLU:HA   | 5        | 0.11          |
| (1,867) | 1:15:A:LEU:HD11 | 1:18:A:GLU:HA   | 19       | 0.11          |
| (1,867) | 1:15:A:LEU:HD12 | 1:18:A:GLU:HA   | 19       | 0.11          |
| (1,867) | 1:15:A:LEU:HD13 | 1:18:A:GLU:HA   | 19       | 0.11          |
| (1,864) | 1:69:A:PHE:HA   | 1:69:A:PHE:HB2  | 18       | 0.11          |
| (1,850) | 1:23:A:ILE:HA   | 1:23:A:ILE:HG13 | 3        | 0.11          |
| (1,850) | 1:23:A:ILE:HA   | 1:23:A:ILE:HG13 | 5        | 0.11          |
| (1,753) | 1:50:A:LEU:H    | 1:50:A:LEU:HD21 | 11       | 0.11          |
| (1,753) | 1:50:A:LEU:H    | 1:50:A:LEU:HD22 | 11       | 0.11          |
| (1,753) | 1:50:A:LEU:H    | 1:50:A:LEU:HD23 | 11       | 0.11          |
| (1,745) | 1:50:A:LEU:HA   | 1:50:A:LEU:HD11 | 11       | 0.11          |
| (1,745) | 1:50:A:LEU:HA   | 1:50:A:LEU:HD12 | 11       | 0.11          |
| (1,745) | 1:50:A:LEU:HA   | 1:50:A:LEU:HD13 | 11       | 0.11          |
| (1,741) | 1:15:A:LEU:HG   | 1:16:A:CYS:HA   | 1        | 0.11          |
| (1,741) | 1:15:A:LEU:HG   | 1:16:A:CYS:HA   | 4        | 0.11          |
| (1,741) | 1:15:A:LEU:HG   | 1:16:A:CYS:HA   | 9        | 0.11          |
| (1,741) | 1:15:A:LEU:HG   | 1:16:A:CYS:HA   | 12       | 0.11          |
| (1,741) | 1:15:A:LEU:HG   | 1:16:A:CYS:HA   | 19       | 0.11          |
| (1,734) | 1:27:A:ILE:H    | 1:27:A:ILE:HG21 | 2        | 0.11          |
| (1,734) | 1:27:A:ILE:H    | 1:27:A:ILE:HG22 | 2        | 0.11          |
| (1,734) | 1:27:A:ILE:H    | 1:27:A:ILE:HG23 | 2        | 0.11          |
| (1,717) | 1:53:A:VAL:HG11 | 1:60:A:TYR:HB3  | 14       | 0.11          |
| (1,717) | 1:53:A:VAL:HG12 | 1:60:A:TYR:HB3  | 14       | 0.11          |
| (1,717) | 1:53:A:VAL:HG13 | 1:60:A:TYR:HB3  | 14       | 0.11          |
| (1,717) | 1:53:A:VAL:HG21 | 1:60:A:TYR:HB3  | 14       | 0.11          |
| (1,717) | 1:53:A:VAL:HG22 | 1:60:A:TYR:HB3  | 14       | 0.11          |
| (1,717) | 1:53:A:VAL:HG23 | 1:60:A:TYR:HB3  | 14       | 0.11          |
| (1,706) | 1:23:A:ILE:HA   | 1:23:A:ILE:HD11 | 2        | 0.11          |
| (1,706) | 1:23:A:ILE:HA   | 1:23:A:ILE:HD12 | 2        | 0.11          |
| (1,706) | 1:23:A:ILE:HA   | 1:23:A:ILE:HD13 | 2        | 0.11          |
| (1,706) | 1:23:A:ILE:HA   | 1:23:A:ILE:HD11 | 16       | 0.11          |
| (1,706) | 1:23:A:ILE:HA   | 1:23:A:ILE:HD12 | 16       | 0.11          |
| (1,706) | 1:23:A:ILE:HA   | 1:23:A:ILE:HD13 | 16       | 0.11          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD21 | 4        | 0.11          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD22 | 4        | 0.11          |
| (1,700) | 1:19:A:LEU:H    | 1:19:A:LEU:HD23 | 4        | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,668) | 1:38:A:LEU:H    | 1:38:A:LEU:HD11 | 14       | 0.11          |
| (1,668) | 1:38:A:LEU:H    | 1:38:A:LEU:HD12 | 14       | 0.11          |
| (1,668) | 1:38:A:LEU:H    | 1:38:A:LEU:HD13 | 14       | 0.11          |
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD11 | 13       | 0.11          |
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD12 | 13       | 0.11          |
| (1,667) | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD13 | 13       | 0.11          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD11 | 13       | 0.11          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD12 | 13       | 0.11          |
| (1,667) | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD13 | 13       | 0.11          |
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD11 | 13       | 0.11          |
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD12 | 13       | 0.11          |
| (1,667) | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD13 | 13       | 0.11          |
| (1,664) | 1:12:A:LEU:HD11 | 1:15:A:LEU:HB2  | 12       | 0.11          |
| (1,664) | 1:12:A:LEU:HD12 | 1:15:A:LEU:HB2  | 12       | 0.11          |
| (1,664) | 1:12:A:LEU:HD13 | 1:15:A:LEU:HB2  | 12       | 0.11          |
| (1,660) | 1:12:A:LEU:HD11 | 1:61:A:ALA:HA   | 8        | 0.11          |
| (1,660) | 1:12:A:LEU:HD12 | 1:61:A:ALA:HA   | 8        | 0.11          |
| (1,660) | 1:12:A:LEU:HD13 | 1:61:A:ALA:HA   | 8        | 0.11          |
| (1,660) | 1:12:A:LEU:HD11 | 1:61:A:ALA:HA   | 15       | 0.11          |
| (1,660) | 1:12:A:LEU:HD12 | 1:61:A:ALA:HA   | 15       | 0.11          |
| (1,660) | 1:12:A:LEU:HD13 | 1:61:A:ALA:HA   | 15       | 0.11          |
| (1,606) | 1:34:A:LYS:HA   | 1:34:A:LYS:HD3  | 14       | 0.11          |
| (1,599) | 1:37:A:LEU:HA   | 1:38:A:LEU:HB3  | 3        | 0.11          |
| (1,599) | 1:37:A:LEU:HA   | 1:38:A:LEU:HB3  | 17       | 0.11          |
| (1,595) | 1:16:A:CYS:HA   | 1:19:A:LEU:HB3  | 1        | 0.11          |
| (1,595) | 1:16:A:CYS:HA   | 1:19:A:LEU:HB3  | 5        | 0.11          |
| (1,595) | 1:16:A:CYS:HA   | 1:19:A:LEU:HB3  | 6        | 0.11          |
| (1,595) | 1:16:A:CYS:HA   | 1:19:A:LEU:HB3  | 7        | 0.11          |
| (1,595) | 1:16:A:CYS:HA   | 1:19:A:LEU:HB3  | 9        | 0.11          |
| (1,595) | 1:16:A:CYS:HA   | 1:19:A:LEU:HB3  | 13       | 0.11          |
| (1,595) | 1:16:A:CYS:HA   | 1:19:A:LEU:HB3  | 19       | 0.11          |
| (1,590) | 1:13:A:PRO:HB3  | 1:46:A:ALA:HB1  | 3        | 0.11          |
| (1,590) | 1:13:A:PRO:HB3  | 1:46:A:ALA:HB2  | 3        | 0.11          |
| (1,590) | 1:13:A:PRO:HB3  | 1:46:A:ALA:HB3  | 3        | 0.11          |
| (1,590) | 1:13:A:PRO:HB3  | 1:46:A:ALA:HB1  | 4        | 0.11          |
| (1,590) | 1:13:A:PRO:HB3  | 1:46:A:ALA:HB2  | 4        | 0.11          |
| (1,590) | 1:13:A:PRO:HB3  | 1:46:A:ALA:HB3  | 4        | 0.11          |
| (1,590) | 1:13:A:PRO:HB3  | 1:46:A:ALA:HB1  | 9        | 0.11          |
| (1,590) | 1:13:A:PRO:HB3  | 1:46:A:ALA:HB2  | 9        | 0.11          |
| (1,590) | 1:13:A:PRO:HB3  | 1:46:A:ALA:HB3  | 9        | 0.11          |
| (1,590) | 1:13:A:PRO:HB3  | 1:46:A:ALA:HB1  | 17       | 0.11          |
| (1,590) | 1:13:A:PRO:HB3  | 1:46:A:ALA:HB2  | 17       | 0.11          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,590) | 1:13:A:PRO:HB3 | 1:46:A:ALA:HB3 | 17       | 0.11          |
| (1,579) | 1:9:A:PRO:HB3  | 1:15:A:LEU:H   | 11       | 0.11          |
| (1,578) | 1:67:A:LEU:H   | 1:67:A:LEU:HG  | 6        | 0.11          |
| (1,578) | 1:67:A:LEU:H   | 1:67:A:LEU:HG  | 7        | 0.11          |
| (1,578) | 1:67:A:LEU:H   | 1:67:A:LEU:HG  | 17       | 0.11          |
| (1,576) | 1:40:A:ARG:H   | 1:40:A:ARG:HB3 | 2        | 0.11          |
| (1,576) | 1:40:A:ARG:H   | 1:40:A:ARG:HB3 | 8        | 0.11          |
| (1,576) | 1:40:A:ARG:H   | 1:40:A:ARG:HB3 | 16       | 0.11          |
| (1,576) | 1:40:A:ARG:H   | 1:40:A:ARG:HB3 | 17       | 0.11          |
| (1,576) | 1:40:A:ARG:H   | 1:40:A:ARG:HB3 | 19       | 0.11          |
| (1,574) | 1:11:A:LYS:HA  | 1:11:A:LYS:HD2 | 2        | 0.11          |
| (1,574) | 1:11:A:LYS:HA  | 1:11:A:LYS:HD3 | 2        | 0.11          |
| (1,561) | 1:39:A:ARG:HG2 | 1:43:A:TYR:HB2 | 3        | 0.11          |
| (1,561) | 1:39:A:ARG:HG2 | 1:43:A:TYR:HB3 | 3        | 0.11          |
| (1,561) | 1:39:A:ARG:HG3 | 1:43:A:TYR:HB2 | 3        | 0.11          |
| (1,561) | 1:39:A:ARG:HG3 | 1:43:A:TYR:HB3 | 3        | 0.11          |
| (1,561) | 1:39:A:ARG:HG2 | 1:43:A:TYR:HB2 | 12       | 0.11          |
| (1,561) | 1:39:A:ARG:HG2 | 1:43:A:TYR:HB3 | 12       | 0.11          |
| (1,561) | 1:39:A:ARG:HG3 | 1:43:A:TYR:HB2 | 12       | 0.11          |
| (1,561) | 1:39:A:ARG:HG3 | 1:43:A:TYR:HB3 | 12       | 0.11          |
| (1,541) | 1:11:A:LYS:HB2 | 1:13:A:PRO:HD3 | 11       | 0.11          |
| (1,541) | 1:11:A:LYS:HB2 | 1:13:A:PRO:HD3 | 18       | 0.11          |
| (1,541) | 1:11:A:LYS:HB2 | 1:13:A:PRO:HD3 | 20       | 0.11          |
| (1,538) | 1:18:A:GLU:HB3 | 1:19:A:LEU:H   | 12       | 0.11          |
| (1,538) | 1:18:A:GLU:HB3 | 1:19:A:LEU:H   | 15       | 0.11          |
| (1,538) | 1:18:A:GLU:HB3 | 1:19:A:LEU:H   | 18       | 0.11          |
| (1,527) | 1:18:A:GLU:HA  | 1:18:A:GLU:HG3 | 4        | 0.11          |
| (1,518) | 1:40:A:ARG:H   | 1:41:A:GLU:HG2 | 4        | 0.11          |
| (1,518) | 1:40:A:ARG:H   | 1:41:A:GLU:HG2 | 10       | 0.11          |
| (1,510) | 1:22:A:THR:HB  | 1:25:A:ASP:HB2 | 6        | 0.11          |
| (1,510) | 1:22:A:THR:HB  | 1:25:A:ASP:HB2 | 20       | 0.11          |
| (1,493) | 1:65:A:LYS:HB2 | 1:65:A:LYS:HE2 | 14       | 0.11          |
| (1,493) | 1:65:A:LYS:HB2 | 1:65:A:LYS:HE3 | 14       | 0.11          |
| (1,493) | 1:65:A:LYS:HB2 | 1:65:A:LYS:HE2 | 16       | 0.11          |
| (1,493) | 1:65:A:LYS:HB2 | 1:65:A:LYS:HE3 | 16       | 0.11          |
| (1,486) | 1:43:A:TYR:HB2 | 1:47:A:ARG:HB3 | 12       | 0.11          |
| (1,486) | 1:43:A:TYR:HB3 | 1:47:A:ARG:HB3 | 12       | 0.11          |
| (1,486) | 1:43:A:TYR:HB2 | 1:47:A:ARG:HB3 | 15       | 0.11          |
| (1,486) | 1:43:A:TYR:HB3 | 1:47:A:ARG:HB3 | 15       | 0.11          |
| (1,478) | 1:8:A:ARG:HG2  | 1:59:A:PRO:HD2 | 12       | 0.11          |
| (1,478) | 1:8:A:ARG:HG3  | 1:59:A:PRO:HD2 | 12       | 0.11          |
| (1,478) | 1:8:A:ARG:HG2  | 1:59:A:PRO:HD2 | 18       | 0.11          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,478) | 1:8:A:ARG:HG3  | 1:59:A:PRO:HD2 | 18       | 0.11          |
| (1,467) | 1:54:A:TYR:HE1 | 1:58:A:ASN:HA  | 2        | 0.11          |
| (1,467) | 1:54:A:TYR:HE2 | 1:58:A:ASN:HA  | 2        | 0.11          |
| (1,467) | 1:54:A:TYR:HE1 | 1:58:A:ASN:HA  | 3        | 0.11          |
| (1,467) | 1:54:A:TYR:HE2 | 1:58:A:ASN:HA  | 3        | 0.11          |
| (1,467) | 1:54:A:TYR:HE1 | 1:58:A:ASN:HA  | 9        | 0.11          |
| (1,467) | 1:54:A:TYR:HE2 | 1:58:A:ASN:HA  | 9        | 0.11          |
| (1,467) | 1:54:A:TYR:HE1 | 1:58:A:ASN:HA  | 17       | 0.11          |
| (1,467) | 1:54:A:TYR:HE2 | 1:58:A:ASN:HA  | 17       | 0.11          |
| (1,465) | 1:32:A:TYR:HE1 | 1:55:A:ARG:HG2 | 3        | 0.11          |
| (1,465) | 1:32:A:TYR:HE2 | 1:55:A:ARG:HG2 | 3        | 0.11          |
| (1,465) | 1:32:A:TYR:HE1 | 1:55:A:ARG:HG2 | 4        | 0.11          |
| (1,465) | 1:32:A:TYR:HE2 | 1:55:A:ARG:HG2 | 4        | 0.11          |
| (1,465) | 1:32:A:TYR:HE1 | 1:55:A:ARG:HG2 | 20       | 0.11          |
| (1,465) | 1:32:A:TYR:HE2 | 1:55:A:ARG:HG2 | 20       | 0.11          |
| (1,464) | 1:32:A:TYR:HA  | 1:32:A:TYR:HE1 | 1        | 0.11          |
| (1,464) | 1:32:A:TYR:HA  | 1:32:A:TYR:HE2 | 1        | 0.11          |
| (1,464) | 1:32:A:TYR:HA  | 1:32:A:TYR:HE1 | 11       | 0.11          |
| (1,464) | 1:32:A:TYR:HA  | 1:32:A:TYR:HE2 | 11       | 0.11          |
| (1,464) | 1:32:A:TYR:HA  | 1:32:A:TYR:HE1 | 15       | 0.11          |
| (1,464) | 1:32:A:TYR:HA  | 1:32:A:TYR:HE2 | 15       | 0.11          |
| (1,464) | 1:32:A:TYR:HA  | 1:32:A:TYR:HE1 | 18       | 0.11          |
| (1,464) | 1:32:A:TYR:HA  | 1:32:A:TYR:HE2 | 18       | 0.11          |
| (1,461) | 1:70:A:TYR:HA  | 1:70:A:TYR:HE1 | 9        | 0.11          |
| (1,461) | 1:70:A:TYR:HA  | 1:70:A:TYR:HE2 | 9        | 0.11          |
| (1,459) | 1:50:A:LEU:H   | 1:50:A:LEU:HG  | 3        | 0.11          |
| (1,459) | 1:50:A:LEU:H   | 1:50:A:LEU:HG  | 10       | 0.11          |
| (1,455) | 1:54:A:TYR:HD1 | 1:59:A:PRO:HB2 | 5        | 0.11          |
| (1,455) | 1:54:A:TYR:HD2 | 1:59:A:PRO:HB2 | 5        | 0.11          |
| (1,455) | 1:54:A:TYR:HD1 | 1:59:A:PRO:HB2 | 8        | 0.11          |
| (1,455) | 1:54:A:TYR:HD2 | 1:59:A:PRO:HB2 | 8        | 0.11          |
| (1,455) | 1:54:A:TYR:HD1 | 1:59:A:PRO:HB2 | 15       | 0.11          |
| (1,455) | 1:54:A:TYR:HD2 | 1:59:A:PRO:HB2 | 15       | 0.11          |
| (1,455) | 1:54:A:TYR:HD1 | 1:59:A:PRO:HB2 | 18       | 0.11          |
| (1,455) | 1:54:A:TYR:HD2 | 1:59:A:PRO:HB2 | 18       | 0.11          |
| (1,447) | 1:43:A:TYR:H   | 1:43:A:TYR:HE1 | 4        | 0.11          |
| (1,447) | 1:43:A:TYR:H   | 1:43:A:TYR:HE2 | 4        | 0.11          |
| (1,447) | 1:43:A:TYR:H   | 1:43:A:TYR:HE1 | 5        | 0.11          |
| (1,447) | 1:43:A:TYR:H   | 1:43:A:TYR:HE2 | 5        | 0.11          |
| (1,447) | 1:43:A:TYR:H   | 1:43:A:TYR:HE1 | 9        | 0.11          |
| (1,447) | 1:43:A:TYR:H   | 1:43:A:TYR:HE2 | 9        | 0.11          |
| (1,447) | 1:43:A:TYR:H   | 1:43:A:TYR:HE1 | 11       | 0.11          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,447) | 1:43:A:TYR:H   | 1:43:A:TYR:HE2  | 11       | 0.11          |
| (1,447) | 1:43:A:TYR:H   | 1:43:A:TYR:HE1  | 20       | 0.11          |
| (1,447) | 1:43:A:TYR:H   | 1:43:A:TYR:HE2  | 20       | 0.11          |
| (1,424) | 1:30:A:CYS:HA  | 1:60:A:TYR:HD1  | 12       | 0.11          |
| (1,424) | 1:30:A:CYS:HA  | 1:60:A:TYR:HD2  | 12       | 0.11          |
| (1,418) | 1:29:A:GLU:HG2 | 1:60:A:TYR:HD1  | 10       | 0.11          |
| (1,418) | 1:29:A:GLU:HG2 | 1:60:A:TYR:HD2  | 10       | 0.11          |
| (1,418) | 1:29:A:GLU:HG3 | 1:60:A:TYR:HD1  | 10       | 0.11          |
| (1,418) | 1:29:A:GLU:HG3 | 1:60:A:TYR:HD2  | 10       | 0.11          |
| (1,409) | 1:78:A:HIS:HB2 | 1:78:A:HIS:HD2  | 10       | 0.11          |
| (1,409) | 1:78:A:HIS:HB2 | 1:78:A:HIS:HD2  | 17       | 0.11          |
| (1,401) | 1:32:A:TYR:HD1 | 1:55:A:ARG:HG2  | 3        | 0.11          |
| (1,401) | 1:32:A:TYR:HD2 | 1:55:A:ARG:HG2  | 3        | 0.11          |
| (1,401) | 1:32:A:TYR:HD1 | 1:55:A:ARG:HG2  | 11       | 0.11          |
| (1,401) | 1:32:A:TYR:HD2 | 1:55:A:ARG:HG2  | 11       | 0.11          |
| (1,401) | 1:32:A:TYR:HD1 | 1:55:A:ARG:HG2  | 20       | 0.11          |
| (1,401) | 1:32:A:TYR:HD2 | 1:55:A:ARG:HG2  | 20       | 0.11          |
| (1,358) | 1:24:A:HIS:HB3 | 1:24:A:HIS:HD2  | 7        | 0.11          |
| (1,358) | 1:24:A:HIS:HB3 | 1:24:A:HIS:HD2  | 15       | 0.11          |
| (1,358) | 1:24:A:HIS:HB3 | 1:24:A:HIS:HD2  | 16       | 0.11          |
| (1,348) | 1:66:A:CYS:HA  | 1:69:A:PHE:HZ   | 9        | 0.11          |
| (1,339) | 1:57:A:GLY:HA2 | 1:58:A:ASN:HD21 | 18       | 0.11          |
| (1,327) | 1:45:A:PHE:HD1 | 1:61:A:ALA:HA   | 11       | 0.11          |
| (1,327) | 1:45:A:PHE:HD2 | 1:61:A:ALA:HA   | 11       | 0.11          |
| (1,321) | 1:2:A:PHE:HD1  | 1:19:A:LEU:HG   | 12       | 0.11          |
| (1,321) | 1:2:A:PHE:HD2  | 1:19:A:LEU:HG   | 12       | 0.11          |
| (1,317) | 1:24:A:HIS:HB3 | 1:25:A:ASP:H    | 3        | 0.11          |
| (1,317) | 1:24:A:HIS:HB3 | 1:25:A:ASP:H    | 8        | 0.11          |
| (1,317) | 1:24:A:HIS:HB3 | 1:25:A:ASP:H    | 18       | 0.11          |
| (1,316) | 1:2:A:PHE:HD1  | 1:9:A:PRO:HD3   | 14       | 0.11          |
| (1,316) | 1:2:A:PHE:HD2  | 1:9:A:PRO:HD3   | 14       | 0.11          |
| (1,310) | 1:2:A:PHE:HD1  | 1:8:A:ARG:H     | 11       | 0.11          |
| (1,310) | 1:2:A:PHE:HD2  | 1:8:A:ARG:H     | 11       | 0.11          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD11 | 2        | 0.11          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD12 | 2        | 0.11          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD13 | 2        | 0.11          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD11 | 3        | 0.11          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD12 | 3        | 0.11          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD13 | 3        | 0.11          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD11 | 8        | 0.11          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD12 | 8        | 0.11          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD13 | 8        | 0.11          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD11 | 10       | 0.11          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD12 | 10       | 0.11          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD13 | 10       | 0.11          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD11 | 14       | 0.11          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD12 | 14       | 0.11          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD13 | 14       | 0.11          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD11 | 15       | 0.11          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD12 | 15       | 0.11          |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD13 | 15       | 0.11          |
| (1,293) | 1:2:A:PHE:HE1  | 1:9:A:PRO:HD2   | 2        | 0.11          |
| (1,293) | 1:2:A:PHE:HE2  | 1:9:A:PRO:HD2   | 2        | 0.11          |
| (1,292) | 1:2:A:PHE:HA   | 1:2:A:PHE:HE1   | 2        | 0.11          |
| (1,292) | 1:2:A:PHE:HA   | 1:2:A:PHE:HE2   | 2        | 0.11          |
| (1,287) | 1:7:A:GLU:HB2  | 1:8:A:ARG:H     | 6        | 0.11          |
| (1,287) | 1:7:A:GLU:HB2  | 1:8:A:ARG:H     | 10       | 0.11          |
| (1,256) | 1:9:A:PRO:HB3  | 1:11:A:LYS:H    | 2        | 0.11          |
| (1,256) | 1:9:A:PRO:HB3  | 1:11:A:LYS:H    | 10       | 0.11          |
| (1,256) | 1:9:A:PRO:HB3  | 1:11:A:LYS:H    | 14       | 0.11          |
| (1,256) | 1:9:A:PRO:HB3  | 1:11:A:LYS:H    | 19       | 0.11          |
| (1,241) | 1:34:A:LYS:H   | 1:34:A:LYS:HG3  | 2        | 0.11          |
| (1,239) | 1:11:A:LYS:HD2 | 1:14:A:GLN:HE21 | 3        | 0.11          |
| (1,239) | 1:11:A:LYS:HD3 | 1:14:A:GLN:HE21 | 3        | 0.11          |
| (1,216) | 1:46:A:ALA:HB1 | 1:48:A:ARG:H    | 7        | 0.11          |
| (1,216) | 1:46:A:ALA:HB2 | 1:48:A:ARG:H    | 7        | 0.11          |
| (1,216) | 1:46:A:ALA:HB3 | 1:48:A:ARG:H    | 7        | 0.11          |
| (1,178) | 1:3:A:GLN:H    | 1:3:A:GLN:HG2   | 1        | 0.11          |
| (1,178) | 1:3:A:GLN:H    | 1:3:A:GLN:HG3   | 1        | 0.11          |
| (1,167) | 1:74:A:SER:HA  | 1:75:A:GLU:H    | 7        | 0.11          |
| (1,116) | 1:44:A:ASP:H   | 1:44:A:ASP:HB3  | 13       | 0.11          |
| (1,96)  | 1:35:A:GLN:HB2 | 1:36:A:GLN:H    | 11       | 0.11          |
| (1,93)  | 1:29:A:GLU:HA  | 1:36:A:GLN:H    | 8        | 0.11          |
| (1,93)  | 1:29:A:GLU:HA  | 1:36:A:GLN:H    | 11       | 0.11          |
| (1,47)  | 1:54:A:TYR:HD1 | 1:55:A:ARG:H    | 8        | 0.11          |
| (1,47)  | 1:54:A:TYR:HD2 | 1:55:A:ARG:H    | 8        | 0.11          |
| (1,47)  | 1:54:A:TYR:HD1 | 1:55:A:ARG:H    | 19       | 0.11          |
| (1,47)  | 1:54:A:TYR:HD2 | 1:55:A:ARG:H    | 19       | 0.11          |
| (1,45)  | 1:36:A:GLN:HG3 | 1:37:A:LEU:H    | 11       | 0.11          |
| (1,45)  | 1:36:A:GLN:HG3 | 1:37:A:LEU:H    | 14       | 0.11          |
| (1,45)  | 1:36:A:GLN:HG3 | 1:37:A:LEU:H    | 18       | 0.11          |
| (1,26)  | 1:63:A:CYS:H   | 1:66:A:CYS:HB3  | 7        | 0.11          |
| (1,14)  | 1:38:A:LEU:H   | 1:41:A:GLU:HB3  | 7        | 0.11          |
| (1,14)  | 1:38:A:LEU:H   | 1:41:A:GLU:HB3  | 9        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1246) | 1:31:A:VAL:HA   | 1:60:A:TYR:HE1  | 10       | 0.1           |
| (1,1246) | 1:31:A:VAL:HA   | 1:60:A:TYR:HE2  | 10       | 0.1           |
| (1,1234) | 1:10:A:ARG:HA   | 1:52:A:ILE:HD11 | 2        | 0.1           |
| (1,1234) | 1:10:A:ARG:HA   | 1:52:A:ILE:HD12 | 2        | 0.1           |
| (1,1234) | 1:10:A:ARG:HA   | 1:52:A:ILE:HD13 | 2        | 0.1           |
| (1,1232) | 1:24:A:HIS:HA   | 1:43:A:TYR:HE1  | 3        | 0.1           |
| (1,1232) | 1:24:A:HIS:HA   | 1:43:A:TYR:HE2  | 3        | 0.1           |
| (1,1225) | 1:2:A:PHE:HE1   | 1:54:A:TYR:HE1  | 13       | 0.1           |
| (1,1225) | 1:2:A:PHE:HE1   | 1:54:A:TYR:HE2  | 13       | 0.1           |
| (1,1225) | 1:2:A:PHE:HE2   | 1:54:A:TYR:HE1  | 13       | 0.1           |
| (1,1225) | 1:2:A:PHE:HE2   | 1:54:A:TYR:HE2  | 13       | 0.1           |
| (1,1225) | 1:2:A:PHE:HE1   | 1:54:A:TYR:HE1  | 16       | 0.1           |
| (1,1225) | 1:2:A:PHE:HE1   | 1:54:A:TYR:HE2  | 16       | 0.1           |
| (1,1225) | 1:2:A:PHE:HE2   | 1:54:A:TYR:HE1  | 16       | 0.1           |
| (1,1225) | 1:2:A:PHE:HE2   | 1:54:A:TYR:HE2  | 16       | 0.1           |
| (1,1225) | 1:2:A:PHE:HE1   | 1:54:A:TYR:HE1  | 19       | 0.1           |
| (1,1225) | 1:2:A:PHE:HE1   | 1:54:A:TYR:HE2  | 19       | 0.1           |
| (1,1225) | 1:2:A:PHE:HE2   | 1:54:A:TYR:HE1  | 19       | 0.1           |
| (1,1225) | 1:2:A:PHE:HE2   | 1:54:A:TYR:HE2  | 19       | 0.1           |
| (1,1183) | 1:11:A:LYS:H    | 1:11:A:LYS:HB3  | 1        | 0.1           |
| (1,1183) | 1:11:A:LYS:H    | 1:11:A:LYS:HB3  | 16       | 0.1           |
| (1,1183) | 1:11:A:LYS:H    | 1:11:A:LYS:HB3  | 20       | 0.1           |
| (1,1170) | 1:48:A:ARG:H    | 1:48:A:ARG:HD3  | 2        | 0.1           |
| (1,1152) | 1:70:A:TYR:H    | 1:70:A:TYR:HB3  | 12       | 0.1           |
| (1,1140) | 1:29:A:GLU:H    | 1:29:A:GLU:HB2  | 10       | 0.1           |
| (1,1140) | 1:29:A:GLU:H    | 1:29:A:GLU:HB2  | 17       | 0.1           |
| (1,1114) | 1:36:A:GLN:H    | 1:36:A:GLN:HG3  | 17       | 0.1           |
| (1,1106) | 1:10:A:ARG:H    | 1:10:A:ARG:HB3  | 5        | 0.1           |
| (1,1106) | 1:10:A:ARG:H    | 1:10:A:ARG:HB3  | 14       | 0.1           |
| (1,1072) | 1:29:A:GLU:HB2  | 1:37:A:LEU:H    | 5        | 0.1           |
| (1,1064) | 1:26:A:ILE:HD11 | 1:28:A:LEU:HA   | 2        | 0.1           |
| (1,1064) | 1:26:A:ILE:HD12 | 1:28:A:LEU:HA   | 2        | 0.1           |
| (1,1064) | 1:26:A:ILE:HD13 | 1:28:A:LEU:HA   | 2        | 0.1           |
| (1,1064) | 1:26:A:ILE:HD11 | 1:28:A:LEU:HA   | 12       | 0.1           |
| (1,1064) | 1:26:A:ILE:HD12 | 1:28:A:LEU:HA   | 12       | 0.1           |
| (1,1064) | 1:26:A:ILE:HD13 | 1:28:A:LEU:HA   | 12       | 0.1           |
| (1,1064) | 1:26:A:ILE:HD11 | 1:28:A:LEU:HA   | 15       | 0.1           |
| (1,1064) | 1:26:A:ILE:HD12 | 1:28:A:LEU:HA   | 15       | 0.1           |
| (1,1064) | 1:26:A:ILE:HD13 | 1:28:A:LEU:HA   | 15       | 0.1           |
| (1,1064) | 1:26:A:ILE:HD11 | 1:28:A:LEU:HA   | 20       | 0.1           |
| (1,1064) | 1:26:A:ILE:HD12 | 1:28:A:LEU:HA   | 20       | 0.1           |
| (1,1064) | 1:26:A:ILE:HD13 | 1:28:A:LEU:HA   | 20       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1057) | 1:1:A:MET:HE1   | 1:2:A:PHE:HA    | 14       | 0.1           |
| (1,1057) | 1:1:A:MET:HE2   | 1:2:A:PHE:HA    | 14       | 0.1           |
| (1,1057) | 1:1:A:MET:HE3   | 1:2:A:PHE:HA    | 14       | 0.1           |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG11 | 1        | 0.1           |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG12 | 1        | 0.1           |
| (1,1022) | 1:37:A:LEU:HB2  | 1:42:A:VAL:HG13 | 1        | 0.1           |
| (1,984)  | 1:26:A:ILE:HG13 | 1:28:A:LEU:HA   | 14       | 0.1           |
| (1,984)  | 1:26:A:ILE:HG13 | 1:28:A:LEU:HA   | 18       | 0.1           |
| (1,924)  | 1:9:A:PRO:HD2   | 1:15:A:LEU:HB3  | 13       | 0.1           |
| (1,924)  | 1:9:A:PRO:HD2   | 1:15:A:LEU:HB3  | 17       | 0.1           |
| (1,907)  | 1:77:A:ARG:HA   | 1:77:A:ARG:HG2  | 2        | 0.1           |
| (1,907)  | 1:77:A:ARG:HA   | 1:77:A:ARG:HG3  | 2        | 0.1           |
| (1,907)  | 1:77:A:ARG:HA   | 1:77:A:ARG:HG2  | 19       | 0.1           |
| (1,907)  | 1:77:A:ARG:HA   | 1:77:A:ARG:HG3  | 19       | 0.1           |
| (1,867)  | 1:15:A:LEU:HD11 | 1:18:A:GLU:HA   | 13       | 0.1           |
| (1,867)  | 1:15:A:LEU:HD12 | 1:18:A:GLU:HA   | 13       | 0.1           |
| (1,867)  | 1:15:A:LEU:HD13 | 1:18:A:GLU:HA   | 13       | 0.1           |
| (1,741)  | 1:15:A:LEU:HG   | 1:16:A:CYS:HA   | 5        | 0.1           |
| (1,741)  | 1:15:A:LEU:HG   | 1:16:A:CYS:HA   | 11       | 0.1           |
| (1,741)  | 1:15:A:LEU:HG   | 1:16:A:CYS:HA   | 18       | 0.1           |
| (1,734)  | 1:27:A:ILE:H    | 1:27:A:ILE:HG21 | 1        | 0.1           |
| (1,734)  | 1:27:A:ILE:H    | 1:27:A:ILE:HG22 | 1        | 0.1           |
| (1,734)  | 1:27:A:ILE:H    | 1:27:A:ILE:HG23 | 1        | 0.1           |
| (1,667)  | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD11 | 19       | 0.1           |
| (1,667)  | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD12 | 19       | 0.1           |
| (1,667)  | 1:12:A:LEU:HD11 | 1:23:A:ILE:HD13 | 19       | 0.1           |
| (1,667)  | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD11 | 19       | 0.1           |
| (1,667)  | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD12 | 19       | 0.1           |
| (1,667)  | 1:12:A:LEU:HD12 | 1:23:A:ILE:HD13 | 19       | 0.1           |
| (1,667)  | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD11 | 19       | 0.1           |
| (1,667)  | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD12 | 19       | 0.1           |
| (1,667)  | 1:12:A:LEU:HD13 | 1:23:A:ILE:HD13 | 19       | 0.1           |
| (1,664)  | 1:12:A:LEU:HD11 | 1:15:A:LEU:HB2  | 8        | 0.1           |
| (1,664)  | 1:12:A:LEU:HD12 | 1:15:A:LEU:HB2  | 8        | 0.1           |
| (1,664)  | 1:12:A:LEU:HD13 | 1:15:A:LEU:HB2  | 8        | 0.1           |
| (1,664)  | 1:12:A:LEU:HD11 | 1:15:A:LEU:HB2  | 16       | 0.1           |
| (1,664)  | 1:12:A:LEU:HD12 | 1:15:A:LEU:HB2  | 16       | 0.1           |
| (1,664)  | 1:12:A:LEU:HD13 | 1:15:A:LEU:HB2  | 16       | 0.1           |
| (1,664)  | 1:12:A:LEU:HD11 | 1:15:A:LEU:HB2  | 18       | 0.1           |
| (1,664)  | 1:12:A:LEU:HD12 | 1:15:A:LEU:HB2  | 18       | 0.1           |
| (1,664)  | 1:12:A:LEU:HD13 | 1:15:A:LEU:HB2  | 18       | 0.1           |
| (1,660)  | 1:12:A:LEU:HD11 | 1:61:A:ALA:HA   | 19       | 0.1           |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,660) | 1:12:A:LEU:HD12 | 1:61:A:ALA:HA  | 19       | 0.1           |
| (1,660) | 1:12:A:LEU:HD13 | 1:61:A:ALA:HA  | 19       | 0.1           |
| (1,625) | 1:8:A:ARG:HG2   | 1:59:A:PRO:HG2 | 17       | 0.1           |
| (1,625) | 1:8:A:ARG:HG3   | 1:59:A:PRO:HG2 | 17       | 0.1           |
| (1,599) | 1:37:A:LEU:HA   | 1:38:A:LEU:HB3 | 12       | 0.1           |
| (1,599) | 1:37:A:LEU:HA   | 1:38:A:LEU:HB3 | 19       | 0.1           |
| (1,595) | 1:16:A:CYS:HA   | 1:19:A:LEU:HB3 | 3        | 0.1           |
| (1,595) | 1:16:A:CYS:HA   | 1:19:A:LEU:HB3 | 8        | 0.1           |
| (1,584) | 1:22:A:THR:HB   | 1:23:A:ILE:HB  | 17       | 0.1           |
| (1,584) | 1:22:A:THR:HB   | 1:23:A:ILE:HB  | 18       | 0.1           |
| (1,576) | 1:40:A:ARG:H    | 1:40:A:ARG:HB3 | 5        | 0.1           |
| (1,576) | 1:40:A:ARG:H    | 1:40:A:ARG:HB3 | 10       | 0.1           |
| (1,576) | 1:40:A:ARG:H    | 1:40:A:ARG:HB3 | 14       | 0.1           |
| (1,574) | 1:11:A:LYS:HA   | 1:11:A:LYS:HD2 | 1        | 0.1           |
| (1,574) | 1:11:A:LYS:HA   | 1:11:A:LYS:HD3 | 1        | 0.1           |
| (1,561) | 1:39:A:ARG:HG2  | 1:43:A:TYR:HB2 | 5        | 0.1           |
| (1,561) | 1:39:A:ARG:HG2  | 1:43:A:TYR:HB3 | 5        | 0.1           |
| (1,561) | 1:39:A:ARG:HG3  | 1:43:A:TYR:HB2 | 5        | 0.1           |
| (1,561) | 1:39:A:ARG:HG3  | 1:43:A:TYR:HB3 | 5        | 0.1           |
| (1,561) | 1:39:A:ARG:HG2  | 1:43:A:TYR:HB2 | 6        | 0.1           |
| (1,561) | 1:39:A:ARG:HG2  | 1:43:A:TYR:HB3 | 6        | 0.1           |
| (1,561) | 1:39:A:ARG:HG3  | 1:43:A:TYR:HB2 | 6        | 0.1           |
| (1,561) | 1:39:A:ARG:HG3  | 1:43:A:TYR:HB3 | 6        | 0.1           |
| (1,541) | 1:11:A:LYS:HB2  | 1:13:A:PRO:HD3 | 17       | 0.1           |
| (1,511) | 1:62:A:VAL:HA   | 1:63:A:CYS:HB3 | 13       | 0.1           |
| (1,510) | 1:22:A:THR:HB   | 1:25:A:ASP:HB2 | 1        | 0.1           |
| (1,510) | 1:22:A:THR:HB   | 1:25:A:ASP:HB2 | 15       | 0.1           |
| (1,505) | 1:41:A:GLU:HA   | 1:44:A:ASP:HB3 | 19       | 0.1           |
| (1,491) | 1:31:A:VAL:HG21 | 1:60:A:TYR:HB2 | 5        | 0.1           |
| (1,491) | 1:31:A:VAL:HG22 | 1:60:A:TYR:HB2 | 5        | 0.1           |
| (1,491) | 1:31:A:VAL:HG23 | 1:60:A:TYR:HB2 | 5        | 0.1           |
| (1,486) | 1:43:A:TYR:HB2  | 1:47:A:ARG:HB3 | 6        | 0.1           |
| (1,486) | 1:43:A:TYR:HB3  | 1:47:A:ARG:HB3 | 6        | 0.1           |
| (1,486) | 1:43:A:TYR:HB2  | 1:47:A:ARG:HB3 | 16       | 0.1           |
| (1,486) | 1:43:A:TYR:HB3  | 1:47:A:ARG:HB3 | 16       | 0.1           |
| (1,486) | 1:43:A:TYR:HB2  | 1:47:A:ARG:HB3 | 18       | 0.1           |
| (1,486) | 1:43:A:TYR:HB3  | 1:47:A:ARG:HB3 | 18       | 0.1           |
| (1,464) | 1:32:A:TYR:HA   | 1:32:A:TYR:HE1 | 10       | 0.1           |
| (1,464) | 1:32:A:TYR:HA   | 1:32:A:TYR:HE2 | 10       | 0.1           |
| (1,464) | 1:32:A:TYR:HA   | 1:32:A:TYR:HE1 | 14       | 0.1           |
| (1,464) | 1:32:A:TYR:HA   | 1:32:A:TYR:HE2 | 14       | 0.1           |
| (1,461) | 1:70:A:TYR:HA   | 1:70:A:TYR:HE1 | 12       | 0.1           |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,461) | 1:70:A:TYR:HA  | 1:70:A:TYR:HE2  | 12       | 0.1           |
| (1,461) | 1:70:A:TYR:HA  | 1:70:A:TYR:HE1  | 16       | 0.1           |
| (1,461) | 1:70:A:TYR:HA  | 1:70:A:TYR:HE2  | 16       | 0.1           |
| (1,461) | 1:70:A:TYR:HA  | 1:70:A:TYR:HE1  | 18       | 0.1           |
| (1,461) | 1:70:A:TYR:HA  | 1:70:A:TYR:HE2  | 18       | 0.1           |
| (1,459) | 1:50:A:LEU:H   | 1:50:A:LEU:HG   | 16       | 0.1           |
| (1,455) | 1:54:A:TYR:HD1 | 1:59:A:PRO:HB2  | 6        | 0.1           |
| (1,455) | 1:54:A:TYR:HD2 | 1:59:A:PRO:HB2  | 6        | 0.1           |
| (1,455) | 1:54:A:TYR:HD1 | 1:59:A:PRO:HB2  | 12       | 0.1           |
| (1,455) | 1:54:A:TYR:HD2 | 1:59:A:PRO:HB2  | 12       | 0.1           |
| (1,447) | 1:43:A:TYR:H   | 1:43:A:TYR:HE1  | 6        | 0.1           |
| (1,447) | 1:43:A:TYR:H   | 1:43:A:TYR:HE2  | 6        | 0.1           |
| (1,447) | 1:43:A:TYR:H   | 1:43:A:TYR:HE1  | 17       | 0.1           |
| (1,447) | 1:43:A:TYR:H   | 1:43:A:TYR:HE2  | 17       | 0.1           |
| (1,439) | 1:79:A:TYR:HA  | 1:79:A:TYR:HE1  | 10       | 0.1           |
| (1,439) | 1:79:A:TYR:HA  | 1:79:A:TYR:HE2  | 10       | 0.1           |
| (1,418) | 1:29:A:GLU:HG2 | 1:60:A:TYR:HD1  | 19       | 0.1           |
| (1,418) | 1:29:A:GLU:HG2 | 1:60:A:TYR:HD2  | 19       | 0.1           |
| (1,418) | 1:29:A:GLU:HG3 | 1:60:A:TYR:HD1  | 19       | 0.1           |
| (1,418) | 1:29:A:GLU:HG3 | 1:60:A:TYR:HD2  | 19       | 0.1           |
| (1,389) | 1:76:A:TYR:HD1 | 1:77:A:ARG:HA   | 5        | 0.1           |
| (1,389) | 1:76:A:TYR:HD2 | 1:77:A:ARG:HA   | 5        | 0.1           |
| (1,358) | 1:24:A:HIS:HB3 | 1:24:A:HIS:HD2  | 1        | 0.1           |
| (1,358) | 1:24:A:HIS:HB3 | 1:24:A:HIS:HD2  | 2        | 0.1           |
| (1,358) | 1:24:A:HIS:HB3 | 1:24:A:HIS:HD2  | 8        | 0.1           |
| (1,358) | 1:24:A:HIS:HB3 | 1:24:A:HIS:HD2  | 12       | 0.1           |
| (1,347) | 1:68:A:LYS:HE2 | 1:69:A:PHE:HZ   | 3        | 0.1           |
| (1,347) | 1:68:A:LYS:HE3 | 1:69:A:PHE:HZ   | 3        | 0.1           |
| (1,320) | 1:25:A:ASP:H   | 1:26:A:ILE:HB   | 12       | 0.1           |
| (1,316) | 1:2:A:PHE:HD1  | 1:9:A:PRO:HD3   | 11       | 0.1           |
| (1,316) | 1:2:A:PHE:HD2  | 1:9:A:PRO:HD3   | 11       | 0.1           |
| (1,313) | 1:2:A:PHE:H    | 1:2:A:PHE:HD1   | 3        | 0.1           |
| (1,313) | 1:2:A:PHE:H    | 1:2:A:PHE:HD2   | 3        | 0.1           |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD11 | 9        | 0.1           |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD12 | 9        | 0.1           |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD13 | 9        | 0.1           |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD11 | 18       | 0.1           |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD12 | 18       | 0.1           |
| (1,306) | 1:45:A:PHE:HZ  | 1:52:A:ILE:HD13 | 18       | 0.1           |
| (1,256) | 1:9:A:PRO:HB3  | 1:11:A:LYS:H    | 18       | 0.1           |
| (1,235) | 1:30:A:CYS:HB2 | 1:34:A:LYS:H    | 1        | 0.1           |
| (1,235) | 1:30:A:CYS:HB2 | 1:34:A:LYS:H    | 17       | 0.1           |

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| Key    | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|--------|----------------|----------------|----------|---------------|
| (1,93) | 1:29:A:GLU:HA  | 1:36:A:GLN:H   | 13       | 0.1           |
| (1,45) | 1:36:A:GLN:HG3 | 1:37:A:LEU:H   | 16       | 0.1           |
| (1,26) | 1:63:A:CYS:H   | 1:66:A:CYS:HB3 | 4        | 0.1           |
| (1,14) | 1:38:A:LEU:H   | 1:41:A:GLU:HB3 | 14       | 0.1           |

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

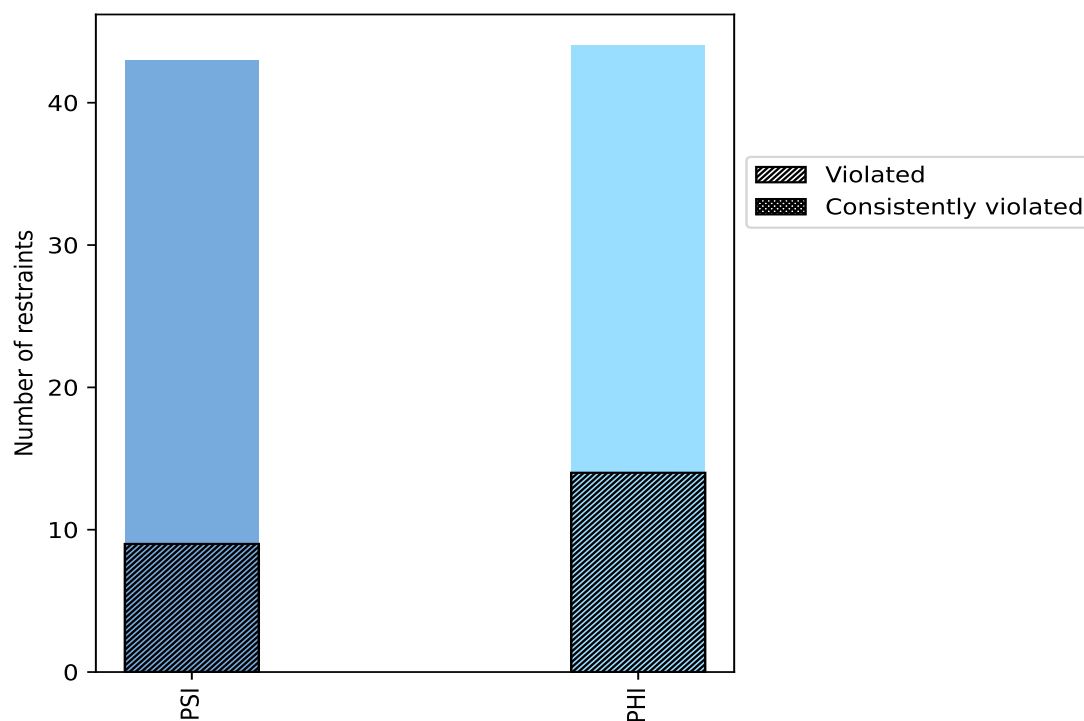
### 10.1 Summary of dihedral-angle violations [i](#)

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> |
| PSI        | 43    | 49.4           | 9                     | 20.9           | 10.3           | 0                                  | 0.0            | 0.0            |
| PHI        | 44    | 50.6           | 14                    | 31.8           | 16.1           | 0                                  | 0.0            | 0.0            |
| Total      | 87    | 100.0          | 23                    | 26.4           | 26.4           | 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](#)



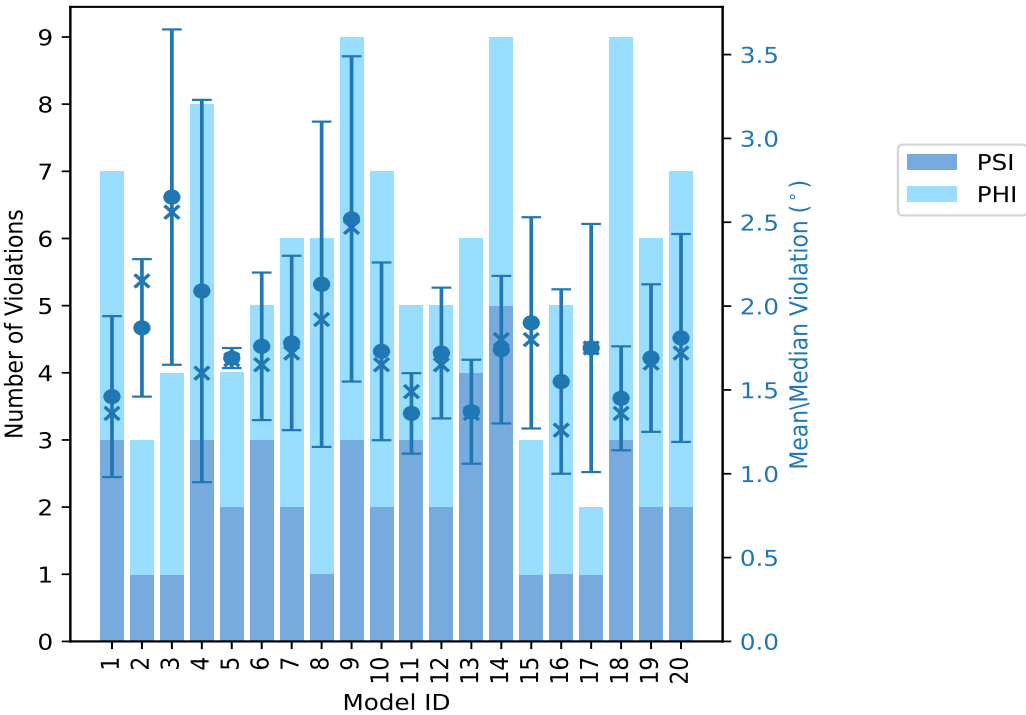
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

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 (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PSI                  | PHI | Total |          |         |        |            |
| 1        | 3                    | 4   | 7     | 1.46     | 2.54    | 0.48   | 1.36       |
| 2        | 1                    | 2   | 3     | 1.87     | 2.17    | 0.41   | 2.15       |
| 3        | 1                    | 3   | 4     | 2.65     | 4.11    | 1.0    | 2.56       |
| 4        | 3                    | 5   | 8     | 2.09     | 4.88    | 1.14   | 1.6        |
| 5        | 2                    | 2   | 4     | 1.69     | 1.78    | 0.06   | 1.68       |
| 6        | 3                    | 2   | 5     | 1.76     | 2.32    | 0.44   | 1.65       |
| 7        | 2                    | 4   | 6     | 1.78     | 2.84    | 0.52   | 1.72       |
| 8        | 1                    | 5   | 6     | 2.13     | 3.85    | 0.97   | 1.92       |
| 9        | 3                    | 6   | 9     | 2.52     | 4.26    | 0.97   | 2.47       |
| 10       | 2                    | 5   | 7     | 1.73     | 2.57    | 0.53   | 1.65       |
| 11       | 3                    | 2   | 5     | 1.36     | 1.63    | 0.24   | 1.49       |
| 12       | 2                    | 3   | 5     | 1.72     | 2.29    | 0.39   | 1.65       |
| 13       | 4                    | 2   | 6     | 1.37     | 1.92    | 0.31   | 1.36       |
| 14       | 5                    | 4   | 9     | 1.74     | 2.54    | 0.44   | 1.8        |
| 15       | 1                    | 2   | 3     | 1.9      | 2.72    | 0.63   | 1.8        |
| 16       | 1                    | 4   | 5     | 1.55     | 2.53    | 0.55   | 1.26       |
| 17       | 1                    | 1   | 2     | 1.75     | 2.49    | 0.74   | 1.75       |
| 18       | 3                    | 6   | 9     | 1.45     | 2.08    | 0.31   | 1.36       |
| 19       | 2                    | 4   | 6     | 1.69     | 2.26    | 0.44   | 1.66       |
| 20       | 2                    | 5   | 7     | 1.81     | 3.14    | 0.62   | 1.72       |

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

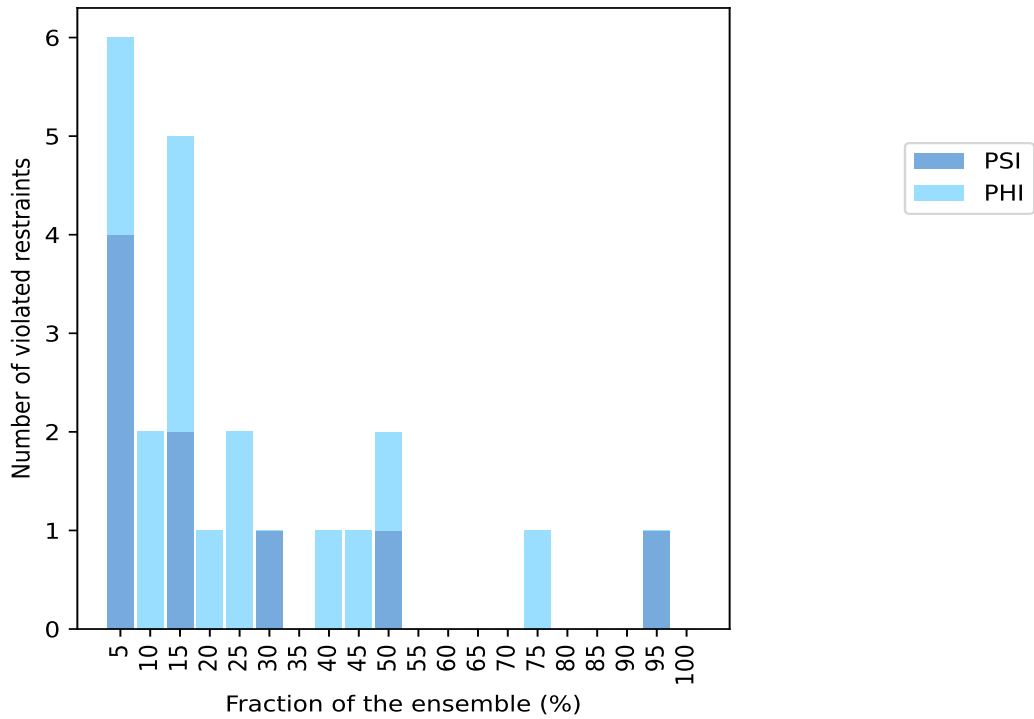
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %     |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

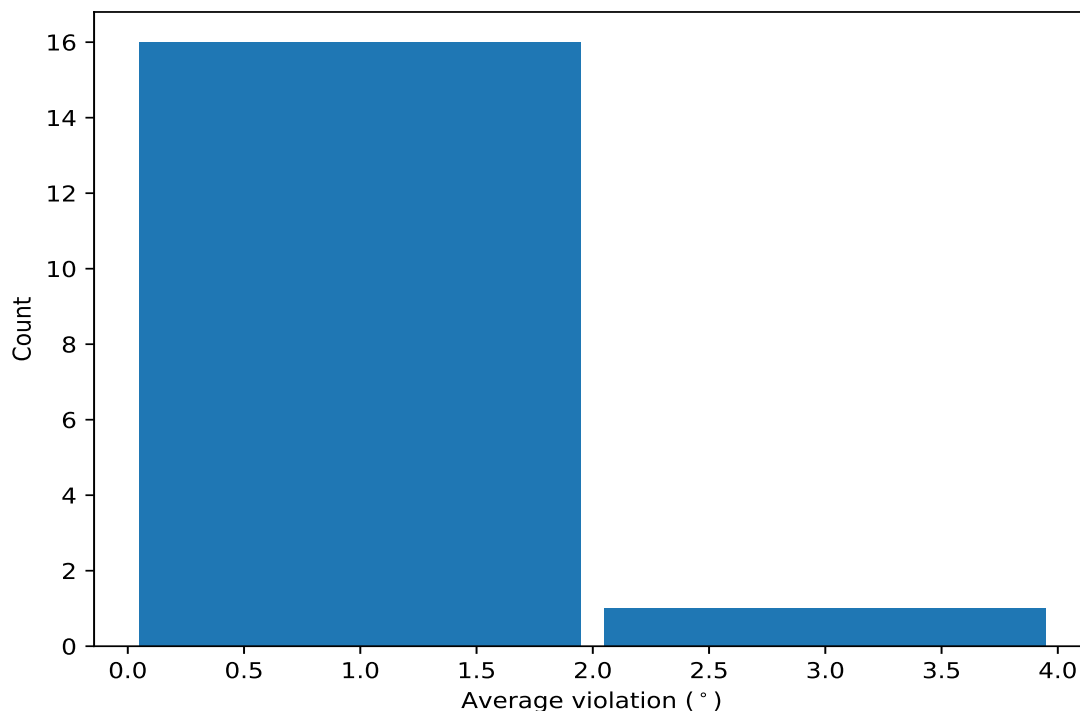


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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.

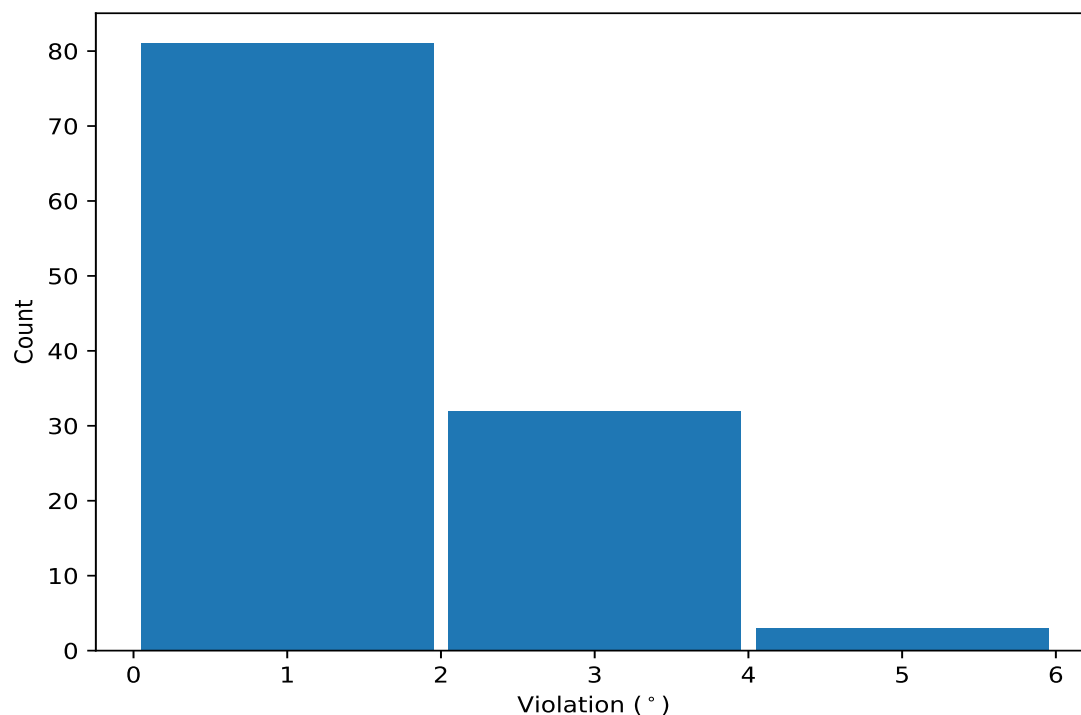
| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|--------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,43) | 1:38:A:LEU:N | 1:38:A:LEU:CA | 1:38:A:LEU:C  | 1:39:A:ARG:N | 19                  | 2.62 | 0.88            | 2.53   |
| (1,58) | 1:45:A:PHE:C | 1:46:A:ALA:N  | 1:46:A:ALA:CA | 1:46:A:ALA:C | 15                  | 1.59 | 0.52            | 1.5    |
| (1,1)  | 1:1:A:MET:C  | 1:2:A:PHE:N   | 1:2:A:PHE:CA  | 1:2:A:PHE:C  | 10                  | 1.94 | 0.62            | 1.72   |
| (1,85) | 1:69:A:PHE:N | 1:69:A:PHE:CA | 1:69:A:PHE:C  | 1:70:A:TYR:N | 10                  | 1.9  | 0.64            | 1.88   |
| (1,60) | 1:51:A:CYS:C | 1:52:A:ILE:N  | 1:52:A:ILE:CA | 1:52:A:ILE:C | 9                   | 1.53 | 0.18            | 1.58   |
| (1,64) | 1:53:A:VAL:C | 1:54:A:TYR:N  | 1:54:A:TYR:CA | 1:54:A:TYR:C | 8                   | 1.43 | 0.38            | 1.32   |
| (1,73) | 1:62:A:VAL:N | 1:62:A:VAL:CA | 1:62:A:VAL:C  | 1:63:A:CYS:N | 6                   | 1.77 | 0.38            | 1.8    |
| (1,44) | 1:38:A:LEU:C | 1:39:A:ARG:N  | 1:39:A:ARG:CA | 1:39:A:ARG:C | 5                   | 1.98 | 0.2             | 2.06   |
| (1,23) | 1:18:A:GLU:C | 1:19:A:LEU:N  | 1:19:A:LEU:CA | 1:19:A:LEU:C | 5                   | 1.25 | 0.24            | 1.2    |
| (1,78) | 1:65:A:LYS:C | 1:66:A:CYS:N  | 1:66:A:CYS:CA | 1:66:A:CYS:C | 4                   | 1.48 | 0.23            | 1.48   |
| (1,4)  | 1:3:A:GLN:N  | 1:3:A:GLN:CA  | 1:3:A:GLN:C   | 1:4:A:ASP:N  | 3                   | 1.76 | 0.63            | 1.61   |
| (1,12) | 1:13:A:PRO:N | 1:13:A:PRO:CA | 1:13:A:PRO:C  | 1:14:A:GLN:N | 3                   | 1.41 | 0.32            | 1.36   |
| (1,5)  | 1:3:A:GLN:C  | 1:4:A:ASP:N   | 1:4:A:ASP:CA  | 1:4:A:ASP:C  | 3                   | 1.35 | 0.22            | 1.26   |
| (1,86) | 1:71:A:SER:C | 1:72:A:LYS:N  | 1:72:A:LYS:CA | 1:72:A:LYS:C | 3                   | 1.23 | 0.12            | 1.28   |
| (1,84) | 1:68:A:LYS:C | 1:69:A:PHE:N  | 1:69:A:PHE:CA | 1:69:A:PHE:C | 3                   | 1.07 | 0.08            | 1.02   |
| (1,3)  | 1:2:A:PHE:C  | 1:3:A:GLN:N   | 1:3:A:GLN:CA  | 1:3:A:GLN:C  | 2                   | 1.87 | 0.6             | 1.87   |
| (1,82) | 1:67:A:LEU:C | 1:68:A:LYS:N  | 1:68:A:LYS:CA | 1:68:A:LYS:C | 2                   | 1.46 | 0.18            | 1.46   |

<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 (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,43) | 1:38:A:LEU:N | 1:38:A:LEU:CA | 1:38:A:LEU:C  | 1:39:A:ARG:N | 4        | 4.88          |
| (1,79) | 1:66:A:CYS:N | 1:66:A:CYS:CA | 1:66:A:CYS:C  | 1:67:A:LEU:N | 9        | 4.26          |
| (1,43) | 1:38:A:LEU:N | 1:38:A:LEU:CA | 1:38:A:LEU:C  | 1:39:A:ARG:N | 3        | 4.11          |
| (1,43) | 1:38:A:LEU:N | 1:38:A:LEU:CA | 1:38:A:LEU:C  | 1:39:A:ARG:N | 8        | 3.85          |
| (1,85) | 1:69:A:PHE:N | 1:69:A:PHE:CA | 1:69:A:PHE:C  | 1:70:A:TYR:N | 9        | 3.3           |
| (1,1)  | 1:1:A:MET:C  | 1:2:A:PHE:N   | 1:2:A:PHE:CA  | 1:2:A:PHE:C  | 9        | 3.29          |
| (1,43) | 1:38:A:LEU:N | 1:38:A:LEU:CA | 1:38:A:LEU:C  | 1:39:A:ARG:N | 20       | 3.14          |
| (1,43) | 1:38:A:LEU:N | 1:38:A:LEU:CA | 1:38:A:LEU:C  | 1:39:A:ARG:N | 9        | 3.12          |
| (1,58) | 1:45:A:PHE:C | 1:46:A:ALA:N  | 1:46:A:ALA:CA | 1:46:A:ALA:C | 3        | 2.85          |
| (1,1)  | 1:1:A:MET:C  | 1:2:A:PHE:N   | 1:2:A:PHE:CA  | 1:2:A:PHE:C  | 8        | 2.85          |
| (1,43) | 1:38:A:LEU:N | 1:38:A:LEU:CA | 1:38:A:LEU:C  | 1:39:A:ARG:N | 7        | 2.84          |
| (1,43) | 1:38:A:LEU:N | 1:38:A:LEU:CA | 1:38:A:LEU:C  | 1:39:A:ARG:N | 15       | 2.72          |
| (1,4)  | 1:3:A:GLN:N  | 1:3:A:GLN:CA  | 1:3:A:GLN:C   | 1:4:A:ASP:N  | 4        | 2.59          |
| (1,58) | 1:45:A:PHE:C | 1:46:A:ALA:N  | 1:46:A:ALA:CA | 1:46:A:ALA:C | 10       | 2.57          |

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| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,43) | 1:38:A:LEU:N | 1:38:A:LEU:CA | 1:38:A:LEU:C  | 1:39:A:ARG:N | 1        | 2.54          |
| (1,43) | 1:38:A:LEU:N | 1:38:A:LEU:CA | 1:38:A:LEU:C  | 1:39:A:ARG:N | 14       | 2.54          |
| (1,43) | 1:38:A:LEU:N | 1:38:A:LEU:CA | 1:38:A:LEU:C  | 1:39:A:ARG:N | 16       | 2.53          |
| (1,43) | 1:38:A:LEU:N | 1:38:A:LEU:CA | 1:38:A:LEU:C  | 1:39:A:ARG:N | 17       | 2.49          |
| (1,3)  | 1:2:A:PHE:C  | 1:3:A:GLN:N   | 1:3:A:GLN:CA  | 1:3:A:GLN:C  | 9        | 2.47          |
| (1,85) | 1:69:A:PHE:N | 1:69:A:PHE:CA | 1:69:A:PHE:C  | 1:70:A:TYR:N | 6        | 2.32          |
| (1,85) | 1:69:A:PHE:N | 1:69:A:PHE:CA | 1:69:A:PHE:C  | 1:70:A:TYR:N | 14       | 2.29          |
| (1,73) | 1:62:A:VAL:N | 1:62:A:VAL:CA | 1:62:A:VAL:C  | 1:63:A:CYS:N | 12       | 2.29          |
| (1,44) | 1:38:A:LEU:C | 1:39:A:ARG:N  | 1:39:A:ARG:CA | 1:39:A:ARG:C | 3        | 2.28          |
| (1,43) | 1:38:A:LEU:N | 1:38:A:LEU:CA | 1:38:A:LEU:C  | 1:39:A:ARG:N | 19       | 2.26          |
| (1,64) | 1:53:A:VAL:C | 1:54:A:TYR:N  | 1:54:A:TYR:CA | 1:54:A:TYR:C | 10       | 2.18          |
| (1,43) | 1:38:A:LEU:N | 1:38:A:LEU:CA | 1:38:A:LEU:C  | 1:39:A:ARG:N | 2        | 2.17          |
| (1,43) | 1:38:A:LEU:N | 1:38:A:LEU:CA | 1:38:A:LEU:C  | 1:39:A:ARG:N | 6        | 2.17          |
| (1,1)  | 1:1:A:MET:C  | 1:2:A:PHE:N   | 1:2:A:PHE:CA  | 1:2:A:PHE:C  | 2        | 2.15          |
| (1,58) | 1:45:A:PHE:C | 1:46:A:ALA:N  | 1:46:A:ALA:CA | 1:46:A:ALA:C | 19       | 2.14          |
| (1,85) | 1:69:A:PHE:N | 1:69:A:PHE:CA | 1:69:A:PHE:C  | 1:70:A:TYR:N | 20       | 2.1           |
| (1,73) | 1:62:A:VAL:N | 1:62:A:VAL:CA | 1:62:A:VAL:C  | 1:63:A:CYS:N | 18       | 2.08          |
| (1,43) | 1:38:A:LEU:N | 1:38:A:LEU:CA | 1:38:A:LEU:C  | 1:39:A:ARG:N | 10       | 2.07          |
| (1,44) | 1:38:A:LEU:C | 1:39:A:ARG:N  | 1:39:A:ARG:CA | 1:39:A:ARG:C | 4        | 2.06          |
| (1,44) | 1:38:A:LEU:C | 1:39:A:ARG:N  | 1:39:A:ARG:CA | 1:39:A:ARG:C | 8        | 2.06          |
| (1,85) | 1:69:A:PHE:N | 1:69:A:PHE:CA | 1:69:A:PHE:C  | 1:70:A:TYR:N | 12       | 2.04          |
| (1,47) | 1:40:A:ARG:N | 1:40:A:ARG:CA | 1:40:A:ARG:C  | 1:41:A:GLU:N | 13       | 1.92          |
| (1,73) | 1:62:A:VAL:N | 1:62:A:VAL:CA | 1:62:A:VAL:C  | 1:63:A:CYS:N | 14       | 1.91          |
| (1,1)  | 1:1:A:MET:C  | 1:2:A:PHE:N   | 1:2:A:PHE:CA  | 1:2:A:PHE:C  | 19       | 1.9           |
| (1,12) | 1:13:A:PRO:N | 1:13:A:PRO:CA | 1:13:A:PRO:C  | 1:14:A:GLN:N | 14       | 1.82          |
| (1,44) | 1:38:A:LEU:C | 1:39:A:ARG:N  | 1:39:A:ARG:CA | 1:39:A:ARG:C | 15       | 1.8           |
| (1,1)  | 1:1:A:MET:C  | 1:2:A:PHE:N   | 1:2:A:PHE:CA  | 1:2:A:PHE:C  | 14       | 1.8           |
| (1,78) | 1:65:A:LYS:C | 1:66:A:CYS:N  | 1:66:A:CYS:CA | 1:66:A:CYS:C | 8        | 1.79          |
| (1,43) | 1:38:A:LEU:N | 1:38:A:LEU:CA | 1:38:A:LEU:C  | 1:39:A:ARG:N | 5        | 1.78          |
| (1,60) | 1:51:A:CYS:C | 1:52:A:ILE:N  | 1:52:A:ILE:CA | 1:52:A:ILE:C | 20       | 1.77          |
| (1,64) | 1:53:A:VAL:C | 1:54:A:TYR:N  | 1:54:A:TYR:CA | 1:54:A:TYR:C | 16       | 1.75          |
| (1,85) | 1:69:A:PHE:N | 1:69:A:PHE:CA | 1:69:A:PHE:C  | 1:70:A:TYR:N | 7        | 1.73          |
| (1,58) | 1:45:A:PHE:C | 1:46:A:ALA:N  | 1:46:A:ALA:CA | 1:46:A:ALA:C | 7        | 1.73          |
| (1,43) | 1:38:A:LEU:N | 1:38:A:LEU:CA | 1:38:A:LEU:C  | 1:39:A:ARG:N | 18       | 1.73          |
| (1,44) | 1:38:A:LEU:C | 1:39:A:ARG:N  | 1:39:A:ARG:CA | 1:39:A:ARG:C | 20       | 1.72          |
| (1,64) | 1:53:A:VAL:C | 1:54:A:TYR:N  | 1:54:A:TYR:CA | 1:54:A:TYR:C | 7        | 1.7           |
| (1,80) | 1:66:A:CYS:C | 1:67:A:LEU:N  | 1:67:A:LEU:CA | 1:67:A:LEU:C | 9        | 1.69          |
| (1,73) | 1:62:A:VAL:N | 1:62:A:VAL:CA | 1:62:A:VAL:C  | 1:63:A:CYS:N | 5        | 1.68          |
| (1,60) | 1:51:A:CYS:C | 1:52:A:ILE:N  | 1:52:A:ILE:CA | 1:52:A:ILE:C | 5        | 1.68          |
| (1,23) | 1:18:A:GLU:C | 1:19:A:LEU:N  | 1:19:A:LEU:CA | 1:19:A:LEU:C | 4        | 1.68          |
| (1,82) | 1:67:A:LEU:C | 1:68:A:LYS:N  | 1:68:A:LYS:CA | 1:68:A:LYS:C | 10       | 1.65          |
| (1,60) | 1:51:A:CYS:C | 1:52:A:ILE:N  | 1:52:A:ILE:CA | 1:52:A:ILE:C | 6        | 1.65          |
| (1,60) | 1:51:A:CYS:C | 1:52:A:ILE:N  | 1:52:A:ILE:CA | 1:52:A:ILE:C | 18       | 1.65          |
| (1,5)  | 1:3:A:GLN:C  | 1:4:A:ASP:N   | 1:4:A:ASP:CA  | 1:4:A:ASP:C  | 12       | 1.65          |
| (1,1)  | 1:1:A:MET:C  | 1:2:A:PHE:N   | 1:2:A:PHE:CA  | 1:2:A:PHE:C  | 1        | 1.63          |
| (1,1)  | 1:1:A:MET:C  | 1:2:A:PHE:N   | 1:2:A:PHE:CA  | 1:2:A:PHE:C  | 11       | 1.63          |
| (1,58) | 1:45:A:PHE:C | 1:46:A:ALA:N  | 1:46:A:ALA:CA | 1:46:A:ALA:C | 5        | 1.61          |
| (1,4)  | 1:3:A:GLN:N  | 1:3:A:GLN:CA  | 1:3:A:GLN:C   | 1:4:A:ASP:N  | 14       | 1.61          |
| (1,60) | 1:51:A:CYS:C | 1:52:A:ILE:N  | 1:52:A:ILE:CA | 1:52:A:ILE:C | 9        | 1.58          |
| (1,58) | 1:45:A:PHE:C | 1:46:A:ALA:N  | 1:46:A:ALA:CA | 1:46:A:ALA:C | 20       | 1.58          |
| (1,78) | 1:65:A:LYS:C | 1:66:A:CYS:N  | 1:66:A:CYS:CA | 1:66:A:CYS:C | 9        | 1.57          |

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| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,85) | 1:69:A:PHE:N | 1:69:A:PHE:CA | 1:69:A:PHE:C  | 1:70:A:TYR:N | 4        | 1.53          |
| (1,73) | 1:62:A:VAL:N | 1:62:A:VAL:CA | 1:62:A:VAL:C  | 1:63:A:CYS:N | 13       | 1.53          |
| (1,85) | 1:69:A:PHE:N | 1:69:A:PHE:CA | 1:69:A:PHE:C  | 1:70:A:TYR:N | 11       | 1.52          |
| (1,58) | 1:45:A:PHE:C | 1:46:A:ALA:N  | 1:46:A:ALA:CA | 1:46:A:ALA:C | 6        | 1.52          |
| (1,54) | 1:43:A:TYR:C | 1:44:A:ASP:N  | 1:44:A:ASP:CA | 1:44:A:ASP:C | 10       | 1.51          |
| (1,60) | 1:51:A:CYS:C | 1:52:A:ILE:N  | 1:52:A:ILE:CA | 1:52:A:ILE:C | 7        | 1.5           |
| (1,58) | 1:45:A:PHE:C | 1:46:A:ALA:N  | 1:46:A:ALA:CA | 1:46:A:ALA:C | 18       | 1.5           |
| (1,43) | 1:38:A:LEU:N | 1:38:A:LEU:CA | 1:38:A:LEU:C  | 1:39:A:ARG:N | 11       | 1.49          |
| (1,1)  | 1:1:A:MET:C  | 1:2:A:PHE:N   | 1:2:A:PHE:CA  | 1:2:A:PHE:C  | 4        | 1.45          |
| (1,60) | 1:51:A:CYS:C | 1:52:A:ILE:N  | 1:52:A:ILE:CA | 1:52:A:ILE:C | 4        | 1.42          |
| (1,60) | 1:51:A:CYS:C | 1:52:A:ILE:N  | 1:52:A:ILE:CA | 1:52:A:ILE:C | 19       | 1.42          |
| (1,58) | 1:45:A:PHE:C | 1:46:A:ALA:N  | 1:46:A:ALA:CA | 1:46:A:ALA:C | 13       | 1.42          |
| (1,78) | 1:65:A:LYS:C | 1:66:A:CYS:N  | 1:66:A:CYS:CA | 1:66:A:CYS:C | 19       | 1.39          |
| (1,57) | 1:45:A:PHE:N | 1:45:A:PHE:CA | 1:45:A:PHE:C  | 1:46:A:ALA:N | 1        | 1.39          |
| (1,64) | 1:53:A:VAL:C | 1:54:A:TYR:N  | 1:54:A:TYR:CA | 1:54:A:TYR:C | 18       | 1.36          |
| (1,58) | 1:45:A:PHE:C | 1:46:A:ALA:N  | 1:46:A:ALA:CA | 1:46:A:ALA:C | 9        | 1.36          |
| (1,12) | 1:13:A:PRO:N | 1:13:A:PRO:CA | 1:13:A:PRO:C  | 1:14:A:GLN:N | 1        | 1.36          |
| (1,86) | 1:71:A:SER:C | 1:72:A:LYS:N  | 1:72:A:LYS:CA | 1:72:A:LYS:C | 14       | 1.35          |
| (1,1)  | 1:1:A:MET:C  | 1:2:A:PHE:N   | 1:2:A:PHE:CA  | 1:2:A:PHE:C  | 3        | 1.35          |
| (1,1)  | 1:1:A:MET:C  | 1:2:A:PHE:N   | 1:2:A:PHE:CA  | 1:2:A:PHE:C  | 12       | 1.35          |
| (1,58) | 1:45:A:PHE:C | 1:46:A:ALA:N  | 1:46:A:ALA:CA | 1:46:A:ALA:C | 2        | 1.3           |
| (1,43) | 1:38:A:LEU:N | 1:38:A:LEU:CA | 1:38:A:LEU:C  | 1:39:A:ARG:N | 13       | 1.29          |
| (1,23) | 1:18:A:GLU:C | 1:19:A:LEU:N  | 1:19:A:LEU:CA | 1:19:A:LEU:C | 18       | 1.29          |
| (1,86) | 1:71:A:SER:C | 1:72:A:LYS:N  | 1:72:A:LYS:CA | 1:72:A:LYS:C | 12       | 1.28          |
| (1,82) | 1:67:A:LEU:C | 1:68:A:LYS:N  | 1:68:A:LYS:CA | 1:68:A:LYS:C | 20       | 1.28          |
| (1,64) | 1:53:A:VAL:C | 1:54:A:TYR:N  | 1:54:A:TYR:CA | 1:54:A:TYR:C | 14       | 1.27          |
| (1,3)  | 1:2:A:PHE:C  | 1:3:A:GLN:N   | 1:3:A:GLN:CA  | 1:3:A:GLN:C  | 18       | 1.27          |
| (1,5)  | 1:3:A:GLN:C  | 1:4:A:ASP:N   | 1:4:A:ASP:CA  | 1:4:A:ASP:C  | 16       | 1.26          |
| (1,23) | 1:18:A:GLU:C | 1:19:A:LEU:N  | 1:19:A:LEU:CA | 1:19:A:LEU:C | 16       | 1.2           |
| (1,84) | 1:68:A:LYS:C | 1:69:A:PHE:N  | 1:69:A:PHE:CA | 1:69:A:PHE:C | 15       | 1.18          |
| (1,78) | 1:65:A:LYS:C | 1:66:A:CYS:N  | 1:66:A:CYS:CA | 1:66:A:CYS:C | 7        | 1.16          |
| (1,60) | 1:51:A:CYS:C | 1:52:A:ILE:N  | 1:52:A:ILE:CA | 1:52:A:ILE:C | 8        | 1.14          |
| (1,5)  | 1:3:A:GLN:C  | 1:4:A:ASP:N   | 1:4:A:ASP:CA  | 1:4:A:ASP:C  | 1        | 1.14          |
| (1,2)  | 1:2:A:PHE:N  | 1:2:A:PHE:CA  | 1:2:A:PHE:C   | 1:3:A:GLN:N  | 11       | 1.13          |
| (1,73) | 1:62:A:VAL:N | 1:62:A:VAL:CA | 1:62:A:VAL:C  | 1:63:A:CYS:N | 6        | 1.12          |
| (1,64) | 1:53:A:VAL:C | 1:54:A:TYR:N  | 1:54:A:TYR:CA | 1:54:A:TYR:C | 4        | 1.12          |
| (1,58) | 1:45:A:PHE:C | 1:46:A:ALA:N  | 1:46:A:ALA:CA | 1:46:A:ALA:C | 1        | 1.11          |
| (1,58) | 1:45:A:PHE:C | 1:46:A:ALA:N  | 1:46:A:ALA:CA | 1:46:A:ALA:C | 8        | 1.11          |
| (1,58) | 1:45:A:PHE:C | 1:46:A:ALA:N  | 1:46:A:ALA:CA | 1:46:A:ALA:C | 14       | 1.11          |
| (1,85) | 1:69:A:PHE:N | 1:69:A:PHE:CA | 1:69:A:PHE:C  | 1:70:A:TYR:N | 10       | 1.09          |
| (1,64) | 1:53:A:VAL:C | 1:54:A:TYR:N  | 1:54:A:TYR:CA | 1:54:A:TYR:C | 20       | 1.08          |
| (1,4)  | 1:3:A:GLN:N  | 1:3:A:GLN:CA  | 1:3:A:GLN:C   | 1:4:A:ASP:N  | 18       | 1.08          |
| (1,86) | 1:71:A:SER:C | 1:72:A:LYS:N  | 1:72:A:LYS:CA | 1:72:A:LYS:C | 18       | 1.07          |
| (1,85) | 1:69:A:PHE:N | 1:69:A:PHE:CA | 1:69:A:PHE:C  | 1:70:A:TYR:N | 19       | 1.05          |
| (1,23) | 1:18:A:GLU:C | 1:19:A:LEU:N  | 1:19:A:LEU:CA | 1:19:A:LEU:C | 10       | 1.04          |
| (1,12) | 1:13:A:PRO:N | 1:13:A:PRO:CA | 1:13:A:PRO:C  | 1:14:A:GLN:N | 13       | 1.04          |
| (1,84) | 1:68:A:LYS:C | 1:69:A:PHE:N  | 1:69:A:PHE:CA | 1:69:A:PHE:C | 1        | 1.02          |
| (1,23) | 1:18:A:GLU:C | 1:19:A:LEU:N  | 1:19:A:LEU:CA | 1:19:A:LEU:C | 13       | 1.02          |
| (1,84) | 1:68:A:LYS:C | 1:69:A:PHE:N  | 1:69:A:PHE:CA | 1:69:A:PHE:C | 16       | 1.01          |
| (1,64) | 1:53:A:VAL:C | 1:54:A:TYR:N  | 1:54:A:TYR:CA | 1:54:A:TYR:C | 11       | 1.01          |
| (1,58) | 1:45:A:PHE:C | 1:46:A:ALA:N  | 1:46:A:ALA:CA | 1:46:A:ALA:C | 17       | 1.01          |