



# Full wwPDB NMR Structure Validation Report ⓘ

Nov 17, 2025 – 06:14 PM JST

PDB ID : 9LS6 / pdb\_00009ls6  
BMRB ID : 36729  
Title : Solution structure of holo Acyl carrier protein 1 (ApeE) of aryl polyene biosynthesis from *Acinetobacter baumannii*  
Authors : Yoo, S.; Lee, C.; Choi, S.; Kim, Y.  
Deposited on : 2025-02-03

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 : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

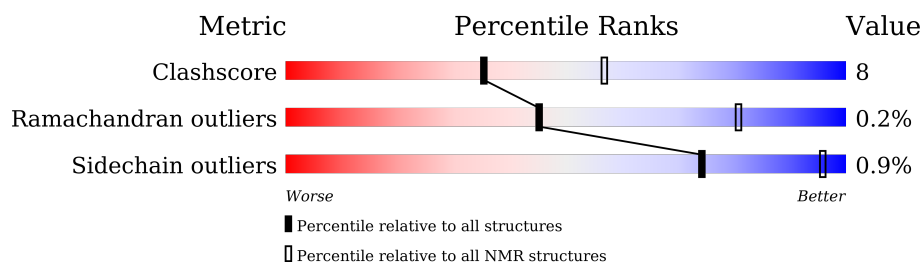
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 86%.

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            | 210492                      | 14027                     |
| Ramachandran outliers | 207382                      | 12486                     |
| Sidechain outliers    | 206894                      | 12463                     |

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     | 86     | <br>74% 15% 10%  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 5 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:3-A:32, A:38-A:84 (77) | 0.19              | 5            |

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 2 clusters. No single-model clusters were found.

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

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1337 atoms, of which 674 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Acyl carrier protein.

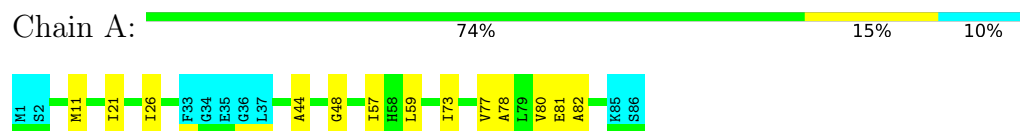
| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 86       | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1337  | 417 | 674 | 107 | 137 | 2 |       |

## 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: Acyl carrier protein

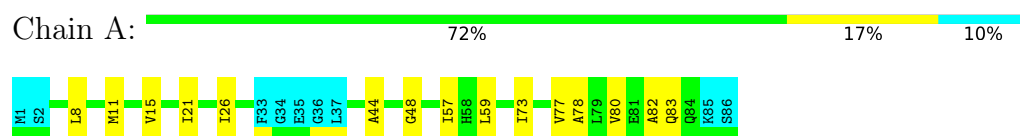


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

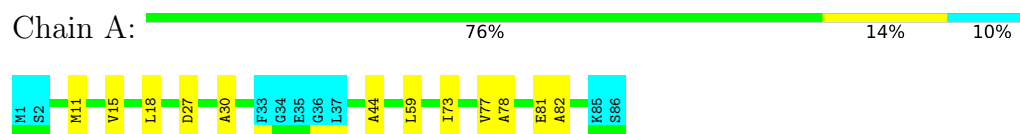
#### 4.2.1 Score per residue for model 1

- Molecule 1: Acyl carrier protein



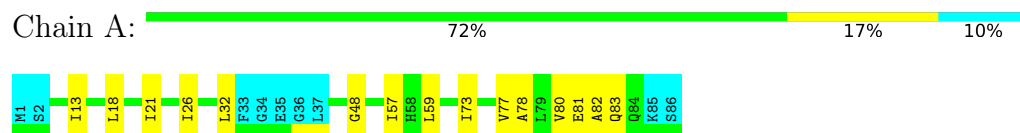
#### 4.2.2 Score per residue for model 2

- Molecule 1: Acyl carrier protein



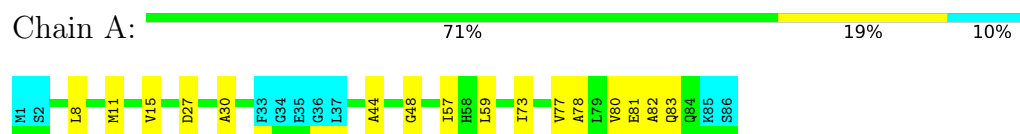
### 4.2.3 Score per residue for model 3

- Molecule 1: Acyl carrier protein



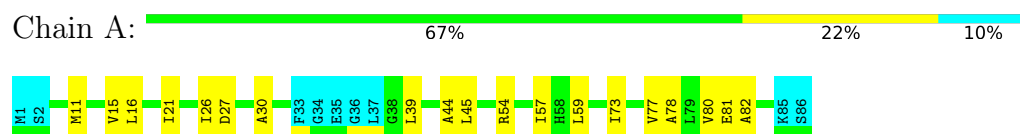
### 4.2.4 Score per residue for model 4

- Molecule 1: Acyl carrier protein



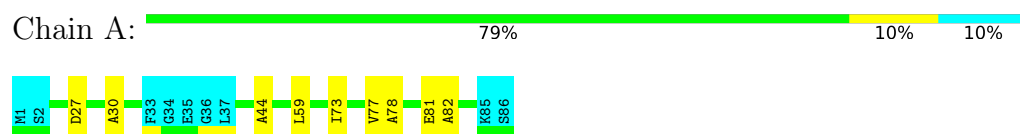
### 4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Acyl carrier protein



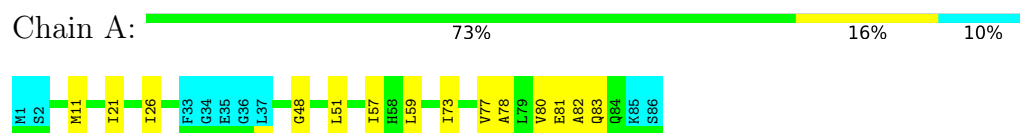
### 4.2.6 Score per residue for model 6

- Molecule 1: Acyl carrier protein



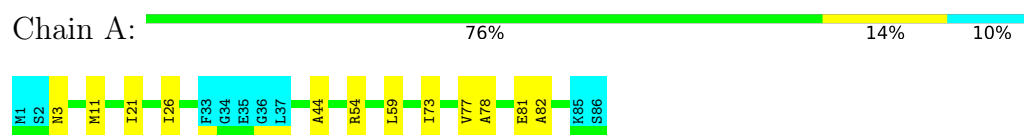
### 4.2.7 Score per residue for model 7

- Molecule 1: Acyl carrier protein



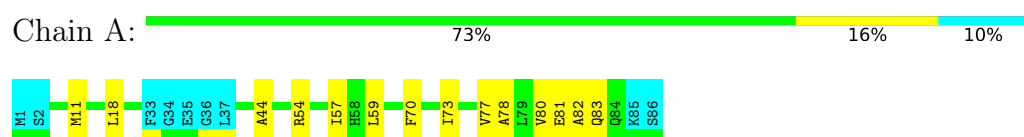
### 4.2.8 Score per residue for model 8

- Molecule 1: Acyl carrier protein



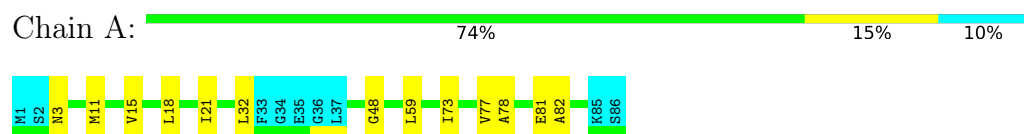
### 4.2.9 Score per residue for model 9

- Molecule 1: Acyl carrier protein



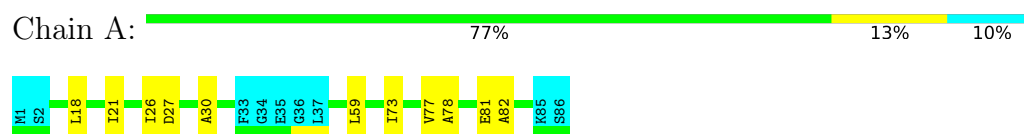
### 4.2.10 Score per residue for model 10

- Molecule 1: Acyl carrier protein



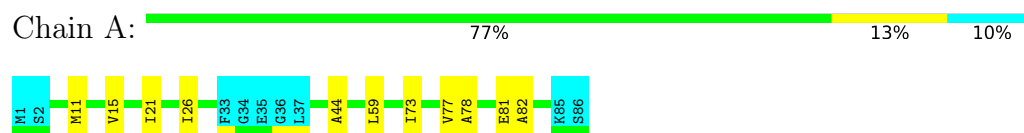
### 4.2.11 Score per residue for model 11

- Molecule 1: Acyl carrier protein



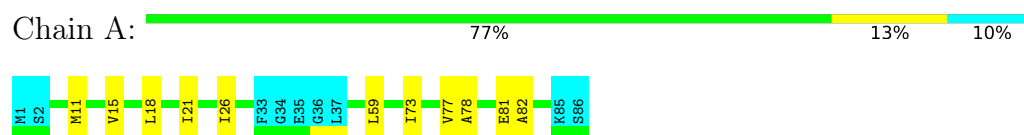
### 4.2.12 Score per residue for model 12

- Molecule 1: Acyl carrier protein



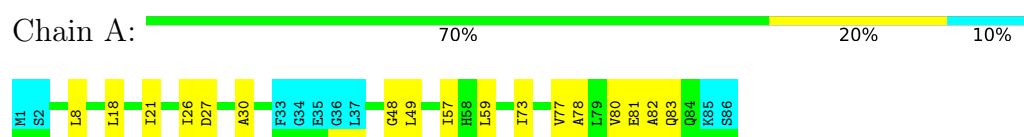
#### 4.2.13 Score per residue for model 13

- Molecule 1: Acyl carrier protein



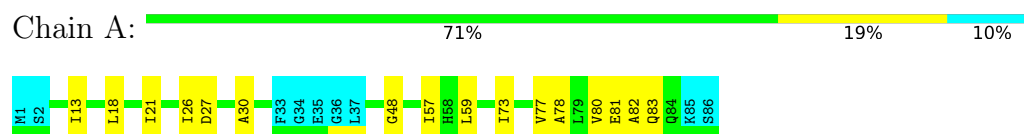
#### 4.2.14 Score per residue for model 14

- Molecule 1: Acyl carrier protein



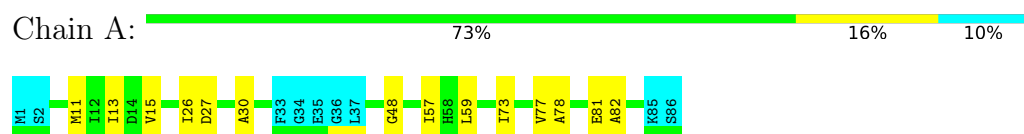
#### 4.2.15 Score per residue for model 15

- Molecule 1: Acyl carrier protein



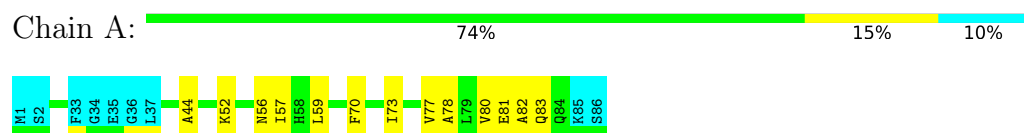
#### 4.2.16 Score per residue for model 16

- Molecule 1: Acyl carrier protein



#### 4.2.17 Score per residue for model 17

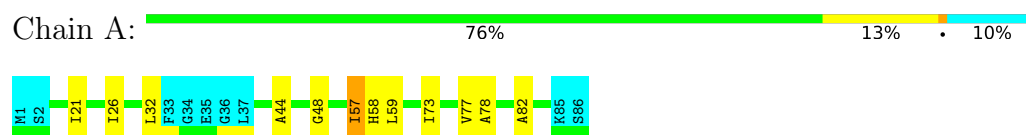
- Molecule 1: Acyl carrier protein





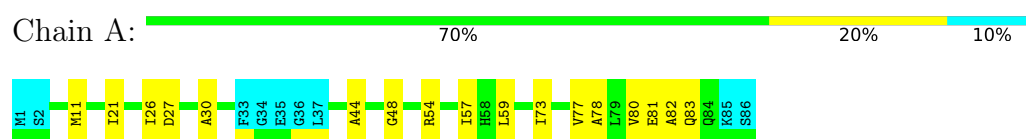
#### 4.2.18 Score per residue for model 18

- Molecule 1: Acyl carrier protein



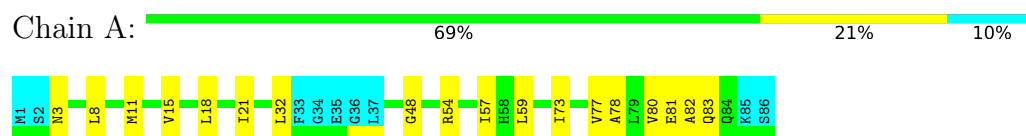
#### 4.2.19 Score per residue for model 19

- Molecule 1: Acyl carrier protein



#### 4.2.20 Score per residue for model 20

- Molecule 1: Acyl carrier protein



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *na*.

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *all calculated structures submitted*.

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| PONDEROSA-C/S | refinement            |         |
| X-PLOR NIH    | structure calculation |         |

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                       | 992            |
| Number of shifts mapped to atoms             | 991            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 1              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 86%            |

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 597   | 608      | 608      | 9±3     |
| All | All   | 11940 | 12160    | 12160    | 186     |

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 8.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:57:ILE:HD13 | 1:A:80:VAL:HG22 | 0.85     | 1.47        | 17     | 10    |
| 1:A:11:MET:HE3  | 1:A:15:VAL:CG2  | 0.69     | 2.17        | 1      | 7     |
| 1:A:59:LEU:O    | 1:A:59:LEU:HD12 | 0.65     | 1.92        | 5      | 16    |
| 1:A:57:ILE:CD1  | 1:A:80:VAL:HG22 | 0.64     | 2.22        | 17     | 10    |
| 1:A:57:ILE:HD12 | 1:A:80:VAL:HG22 | 0.59     | 1.73        | 5      | 1     |
| 1:A:27:ASP:HB2  | 1:A:30:ALA:HB2  | 0.55     | 1.79        | 15     | 9     |
| 1:A:48:GLY:HA3  | 1:A:59:LEU:HD11 | 0.54     | 1.79        | 19     | 8     |
| 1:A:21:ILE:HG21 | 1:A:26:ILE:HD11 | 0.53     | 1.81        | 15     | 11    |
| 1:A:11:MET:HE2  | 1:A:54:ARG:HG3  | 0.51     | 1.83        | 8      | 5     |
| 1:A:21:ILE:CG2  | 1:A:26:ILE:HD11 | 0.50     | 2.35        | 15     | 1     |
| 1:A:49:LEU:HD13 | 1:A:49:LEU:C    | 0.49     | 2.32        | 14     | 1     |
| 1:A:13:ILE:HD11 | 1:A:26:ILE:CG1  | 0.47     | 2.39        | 15     | 1     |
| 1:A:78:ALA:O    | 1:A:82:ALA:HB2  | 0.47     | 2.09        | 20     | 20    |
| 1:A:57:ILE:HD13 | 1:A:58:HIS:N    | 0.45     | 2.26        | 18     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:73:ILE:HD12 | 1:A:73:ILE:N    | 0.44     | 2.28        | 2      | 15    |
| 1:A:73:ILE:O    | 1:A:77:VAL:HG23 | 0.44     | 2.12        | 15     | 15    |
| 1:A:13:ILE:HD11 | 1:A:26:ILE:HG13 | 0.43     | 1.88        | 15     | 1     |
| 1:A:59:LEU:HD13 | 1:A:70:PHE:CZ   | 0.43     | 2.48        | 9      | 2     |
| 1:A:49:LEU:HD13 | 1:A:49:LEU:O    | 0.43     | 2.14        | 14     | 1     |
| 1:A:18:LEU:HB3  | 1:A:21:ILE:HD12 | 0.43     | 1.90        | 10     | 6     |
| 1:A:77:VAL:O    | 1:A:81:GLU:CB   | 0.43     | 2.67        | 15     | 18    |
| 1:A:11:MET:HE1  | 1:A:51:LEU:HA   | 0.42     | 1.91        | 7      | 1     |
| 1:A:48:GLY:CA   | 1:A:59:LEU:HD21 | 0.42     | 2.44        | 16     | 3     |
| 1:A:59:LEU:HD12 | 1:A:59:LEU:C    | 0.42     | 2.40        | 16     | 1     |
| 1:A:11:MET:O    | 1:A:15:VAL:HG23 | 0.41     | 2.15        | 5      | 2     |
| 1:A:8:LEU:HD12  | 1:A:77:VAL:HG22 | 0.41     | 1.91        | 20     | 4     |
| 1:A:13:ILE:CG1  | 1:A:26:ILE:HD12 | 0.41     | 2.45        | 16     | 1     |
| 1:A:13:ILE:HD11 | 1:A:26:ILE:HD12 | 0.41     | 1.93        | 3      | 1     |
| 1:A:73:ILE:HD12 | 1:A:73:ILE:H    | 0.40     | 1.76        | 19     | 6     |
| 1:A:45:LEU:C    | 1:A:45:LEU:HD23 | 0.40     | 2.41        | 5      | 1     |
| 1:A:48:GLY:HA2  | 1:A:59:LEU:HD21 | 0.40     | 1.92        | 16     | 1     |
| 1:A:73:ILE:N    | 1:A:73:ILE:HD12 | 0.40     | 2.31        | 13     | 1     |
| 1:A:48:GLY:CA   | 1:A:59:LEU:HD11 | 0.40     | 2.47        | 15     | 2     |
| 1:A:59:LEU:HD12 | 1:A:59:LEU:O    | 0.40     | 2.16        | 3      | 1     |
| 1:A:52:LYS:O    | 1:A:56:ASN:HA   | 0.40     | 2.16        | 17     | 1     |
| 1:A:16:LEU:HD13 | 1:A:39:LEU:HD21 | 0.40     | 1.92        | 5      | 1     |

## 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed        | Favoured     | Allowed    | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|------------|------------|-------------|----|
| 1   | A     | 77/86 (90%)     | 76±1 (98±1%) | 1±1 (2±1%) | 0±0 (0±0%) | 45          | 81 |
| All | All   | 1540/1720 (90%) | 1510 (98%)   | 27 (2%)    | 3 (0%)     | 45          | 81 |

All 1 unique Ramachandran outliers are listed below.

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

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

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

| Mol | Chain | Analysed        | Rotameric    | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|------------|-------------|----|
| 1   | A     | 66/73 (90%)     | 65±0 (99±1%) | 1±0 (1±1%) | 74          | 96 |
| All | All   | 1320/1460 (90%) | 1308 (99%)   | 12 (1%)    | 74          | 96 |

All 2 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     | 83  | GLN  | 10             |
| 1   | A     | 57  | ILE  | 2              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 86% for the well-defined parts and 85% for the entire structure.

### 7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch\_output*

#### 7.1.1 Bookkeeping

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

|   |     |
|---|-----|
| Total number of shifts                  | 992 |
| Number of shifts mapped to atoms        | 991 |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 1   |
| Number of shifts with mapping warnings  | 0   |
| Number of shift outliers (ShiftChecker) | 0   |

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

- No matching atom found in the structure. All 1 occurrences are reported below.

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 1   | MET  | H    | 8.568      | 0.002       | 1         |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 86       | $-0.35 \pm 0.17$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 82       | $0.10 \pm 0.14$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 84       | $-0.32 \pm 0.22$                | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 85       | $-0.04 \pm 0.65$                | None needed ( $< 0.5$ ppm) |

### 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 86%, i.e. 903 atoms were assigned a chemical shift out of a possible 1053. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|----------------|----------------|-----------------|-----------------|
| Backbone  | 384/385 (100%) | 155/155 (100%) | 153/154 (99%)   | 76/76 (100%)    |
| Sidechain | 512/635 (81%)  | 337/415 (81%)  | 175/204 (86%)   | 0/16 (0%)       |
| Aromatic  | 7/33 (21%)     | 7/17 (41%)     | 0/14 (0%)       | 0/2 (0%)        |
| Overall   | 903/1053 (86%) | 499/587 (85%)  | 328/372 (88%)   | 76/94 (81%)     |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 992 atoms were assigned a chemical shift out of a possible 1162. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|----------------|----------------|-----------------|-----------------|
| Backbone  | 430/432 (100%) | 175/175 (100%) | 170/172 (99%)   | 85/85 (100%)    |
| Sidechain | 553/687 (80%)  | 363/449 (81%)  | 190/221 (86%)   | 0/17 (0%)       |
| Aromatic  | 9/43 (21%)     | 9/22 (41%)     | 0/19 (0%)       | 0/2 (0%)        |
| Overall   | 992/1162 (85%) | 547/646 (85%)  | 360/412 (87%)   | 85/104 (82%)    |

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

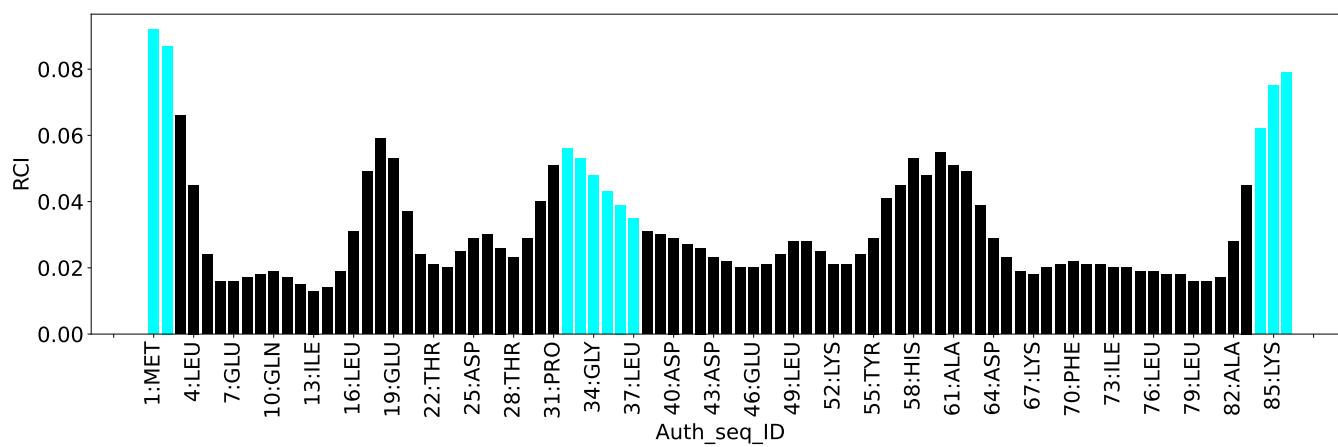
There are no statistically unusual chemical shifts.

### 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                                | 1307  |
| Intra-residue ( $ i-j =0$ )                              | 2     |
| Sequential ( $ i-j =1$ )                                 | 268   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 615   |
| Long range ( $ i-j \geq 5$ )                             | 346   |
| Inter-chain  | 0     |
| Hydrogen bond restraints                                 | 76    |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 145   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 16.9  |
| Number of long range restraints per residue <sup>1</sup> | 4.1   |

<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)  | 91.2                                   | 0.2     |
| 0.2-0.5 (Medium) | 5.0                                    | 0.45    |
| >0.5 (Large)     | 0.1                                    | 0.78    |

### 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)   | 5.3                                    | 5.06    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

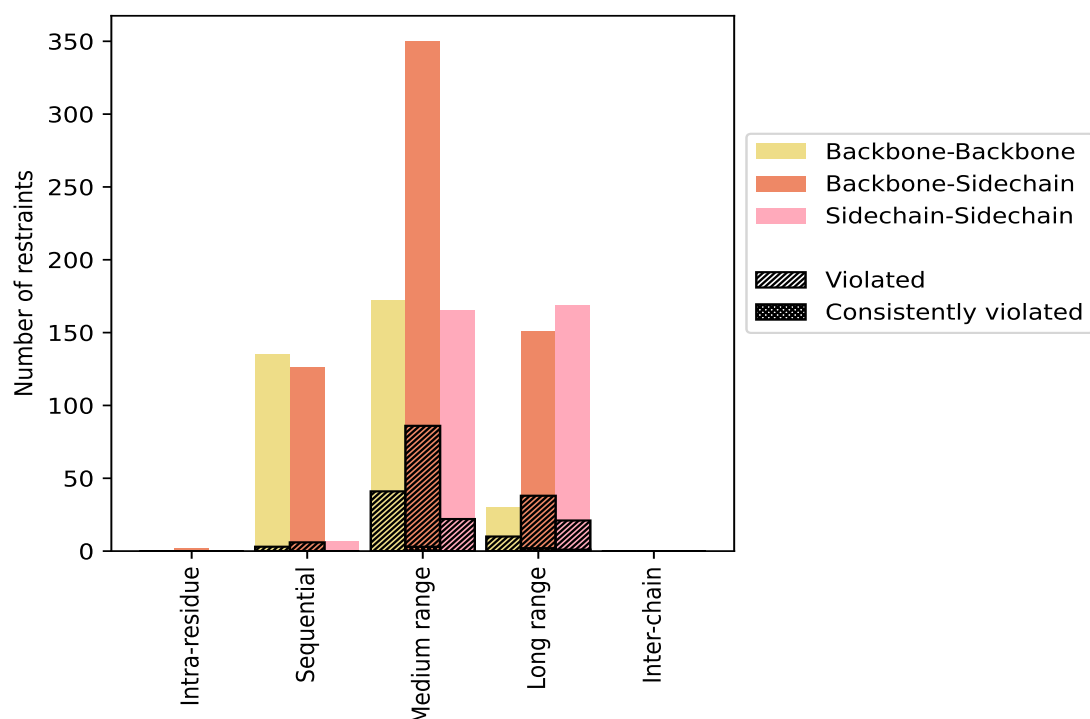
### 9.1 Summary of distance violations ⓘ

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>2</b>    | <b>0.2</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  | 2           | 0.2            | 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>Sequential (<math> i-j =1</math>)</b>                                    | <b>268</b>  | <b>20.5</b>    | <b>9</b>              | <b>3.4</b>     | <b>0.7</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone   | 135         | 10.3           | 3                     | 2.2            | 0.2            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 126         | 9.6            | 6                     | 4.8            | 0.5            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain   | 7           | 0.5            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>615</b>  | <b>47.1</b>    | <b>134</b>            | <b>21.8</b>    | <b>10.3</b>    | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone   | 172         | 13.2           | 41                    | 23.8           | 3.1            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 278         | 21.3           | 71                    | 25.5           | 5.4            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain   | 165         | 12.6           | 22                    | 13.3           | 1.7            | 0                                  | 0.0            | 0.0            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>346</b>  | <b>26.5</b>    | <b>69</b>             | <b>19.9</b>    | <b>5.3</b>     | <b>3</b>                           | <b>0.9</b>     | <b>0.2</b>     |
| Backbone-Backbone   | 30          | 2.3            | 10                    | 33.3           | 0.8            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 147         | 11.2           | 38                    | 25.9           | 2.9            | 2                                  | 1.4            | 0.2            |
| Sidechain-Sidechain   | 169         | 12.9           | 21                    | 12.4           | 1.6            | 1                                  | 0.6            | 0.1            |
| <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>76</b>   | <b>5.8</b>     | <b>15</b>             | <b>19.7</b>    | <b>1.1</b>     | <b>3</b>                           | <b>3.9</b>     | <b>0.2</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>1307</b> | <b>100.0</b>   | <b>227</b>            | <b>17.4</b>    | <b>17.4</b>    | <b>6</b>                           | <b>0.5</b>     | <b>0.5</b>     |
| Backbone-Backbone   | 337         | 25.8           | 54                    | 16.0           | 4.1            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 629         | 48.1           | 130                   | 20.7           | 9.9            | 5                                  | 0.8            | 0.4            |
| Sidechain-Sidechain   | 341         | 26.1           | 43                    | 12.6           | 3.3            | 1                                  | 0.3            | 0.1            |

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

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



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

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 0                    | 3               | 83              | 36              | 0               | 122   | 0.13     | 0.41    | 0.04                | 0.12       |
| 2        | 0                    | 2               | 80              | 34              | 0               | 116   | 0.13     | 0.33    | 0.04                | 0.12       |
| 3        | 0                    | 3               | 78              | 34              | 0               | 115   | 0.13     | 0.44    | 0.05                | 0.12       |
| 4        | 0                    | 2               | 75              | 35              | 0               | 112   | 0.13     | 0.43    | 0.04                | 0.12       |
| 5        | 0                    | 3               | 85              | 33              | 0               | 121   | 0.13     | 0.78    | 0.07                | 0.12       |
| 6        | 0                    | 1               | 90              | 36              | 0               | 127   | 0.13     | 0.35    | 0.03                | 0.11       |
| 7        | 0                    | 2               | 77              | 32              | 0               | 111   | 0.13     | 0.45    | 0.05                | 0.12       |
| 8        | 0                    | 3               | 79              | 28              | 0               | 110   | 0.12     | 0.29    | 0.03                | 0.12       |
| 9        | 0                    | 2               | 79              | 33              | 0               | 114   | 0.13     | 0.68    | 0.07                | 0.11       |
| 10       | 0                    | 4               | 82              | 35              | 0               | 121   | 0.13     | 0.34    | 0.04                | 0.11       |

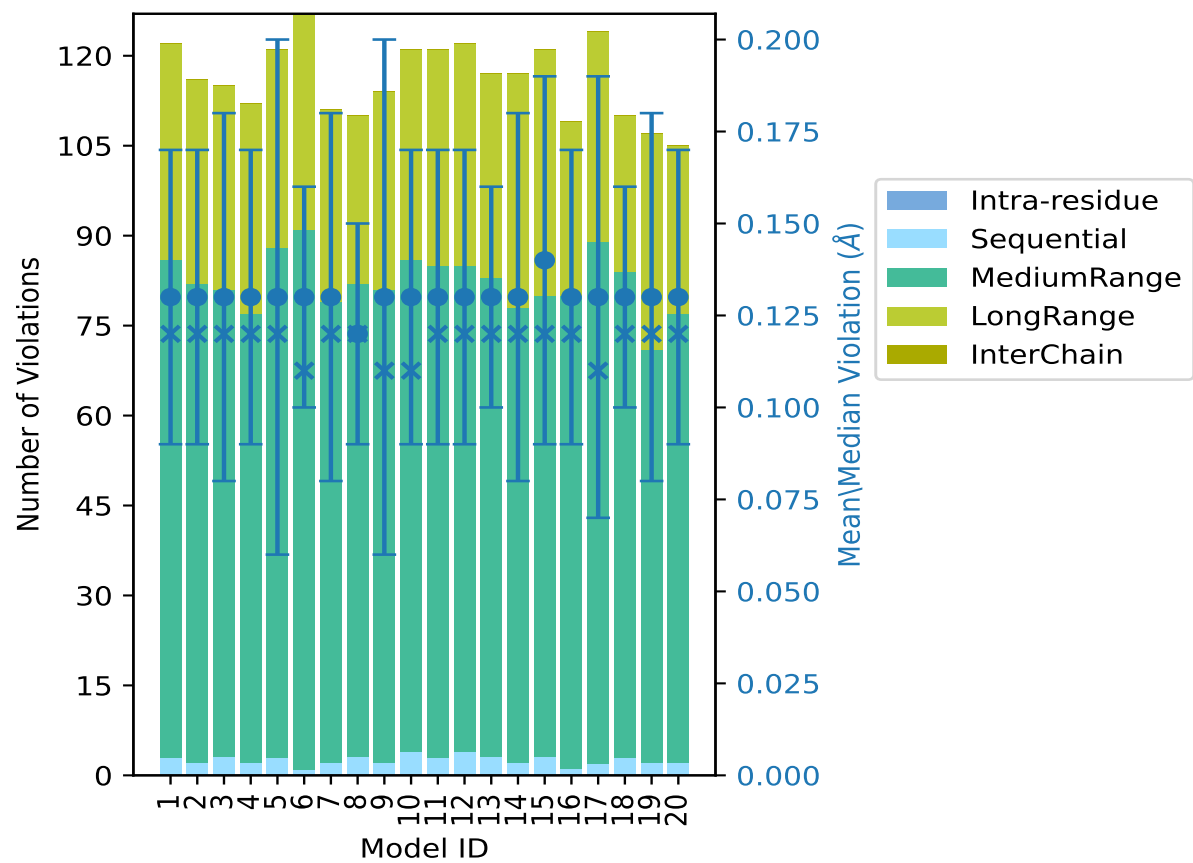
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 0                    | 3               | 82              | 36              | 0               | 121   | 0.13     | 0.34    | 0.04                | 0.12       |
| 12       | 0                    | 4               | 81              | 37              | 0               | 122   | 0.13     | 0.33    | 0.04                | 0.12       |
| 13       | 0                    | 3               | 80              | 34              | 0               | 117   | 0.13     | 0.3     | 0.03                | 0.12       |
| 14       | 0                    | 2               | 76              | 39              | 0               | 117   | 0.13     | 0.43    | 0.05                | 0.12       |
| 15       | 0                    | 3               | 77              | 41              | 0               | 121   | 0.14     | 0.45    | 0.05                | 0.12       |
| 16       | 0                    | 1               | 79              | 29              | 0               | 109   | 0.13     | 0.35    | 0.04                | 0.12       |
| 17       | 0                    | 2               | 87              | 35              | 0               | 124   | 0.13     | 0.63    | 0.06                | 0.11       |
| 18       | 0                    | 3               | 81              | 26              | 0               | 110   | 0.13     | 0.28    | 0.03                | 0.12       |
| 19       | 0                    | 2               | 69              | 36              | 0               | 107   | 0.13     | 0.42    | 0.05                | 0.12       |
| 20       | 0                    | 2               | 75              | 28              | 0               | 105   | 0.13     | 0.45    | 0.04                | 0.12       |

<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

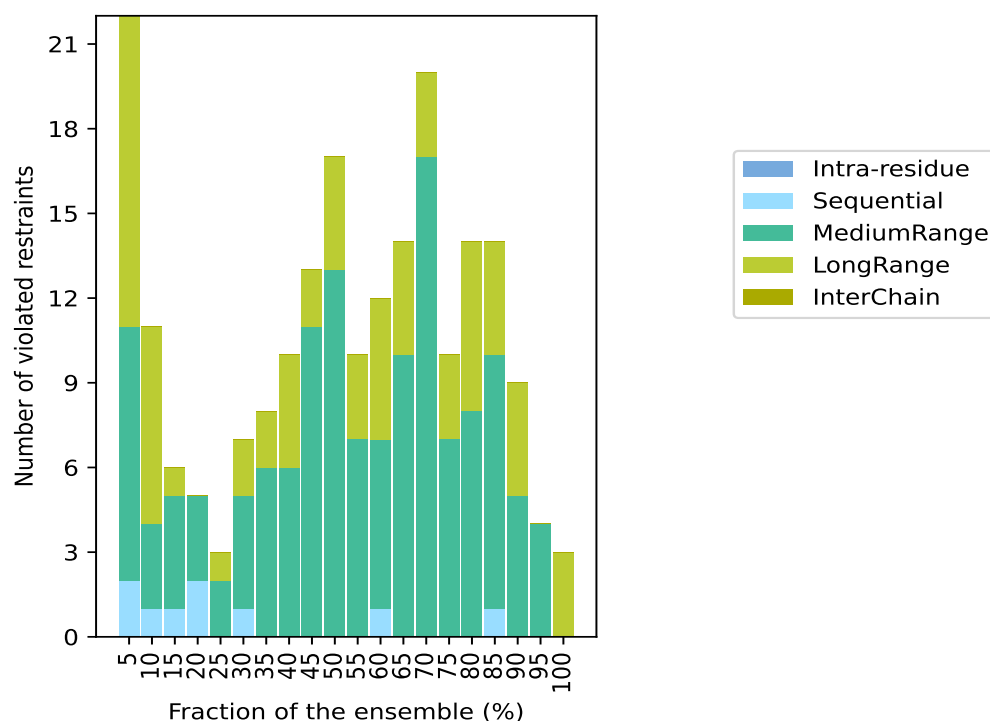
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1019(IR:2, SQ:259, MR:481, LR:277, IC:0) restraints are not 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>       | %     |
| 0                             | 2               | 9               | 11              | 0               | 22    | 1                        | 5.0   |
| 0                             | 1               | 3               | 7               | 0               | 11    | 2                        | 10.0  |
| 0                             | 1               | 4               | 1               | 0               | 6     | 3                        | 15.0  |
| 0                             | 2               | 3               | 0               | 0               | 5     | 4                        | 20.0  |
| 0                             | 0               | 2               | 1               | 0               | 3     | 5                        | 25.0  |
| 0                             | 1               | 4               | 2               | 0               | 7     | 6                        | 30.0  |
| 0                             | 0               | 6               | 2               | 0               | 8     | 7                        | 35.0  |
| 0                             | 0               | 6               | 4               | 0               | 10    | 8                        | 40.0  |
| 0                             | 0               | 11              | 2               | 0               | 13    | 9                        | 45.0  |
| 0                             | 0               | 13              | 4               | 0               | 17    | 10                       | 50.0  |
| 0                             | 0               | 7               | 3               | 0               | 10    | 11                       | 55.0  |
| 0                             | 1               | 6               | 5               | 0               | 12    | 12                       | 60.0  |
| 0                             | 0               | 10              | 4               | 0               | 14    | 13                       | 65.0  |
| 0                             | 0               | 17              | 3               | 0               | 20    | 14                       | 70.0  |
| 0                             | 0               | 7               | 3               | 0               | 10    | 15                       | 75.0  |
| 0                             | 0               | 8               | 6               | 0               | 14    | 16                       | 80.0  |
| 0                             | 1               | 9               | 4               | 0               | 14    | 17                       | 85.0  |
| 0                             | 0               | 5               | 4               | 0               | 9     | 18                       | 90.0  |
| 0                             | 0               | 4               | 0               | 0               | 4     | 19                       | 95.0  |
| 0                             | 0               | 0               | 3               | 0               | 3     | 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](#)

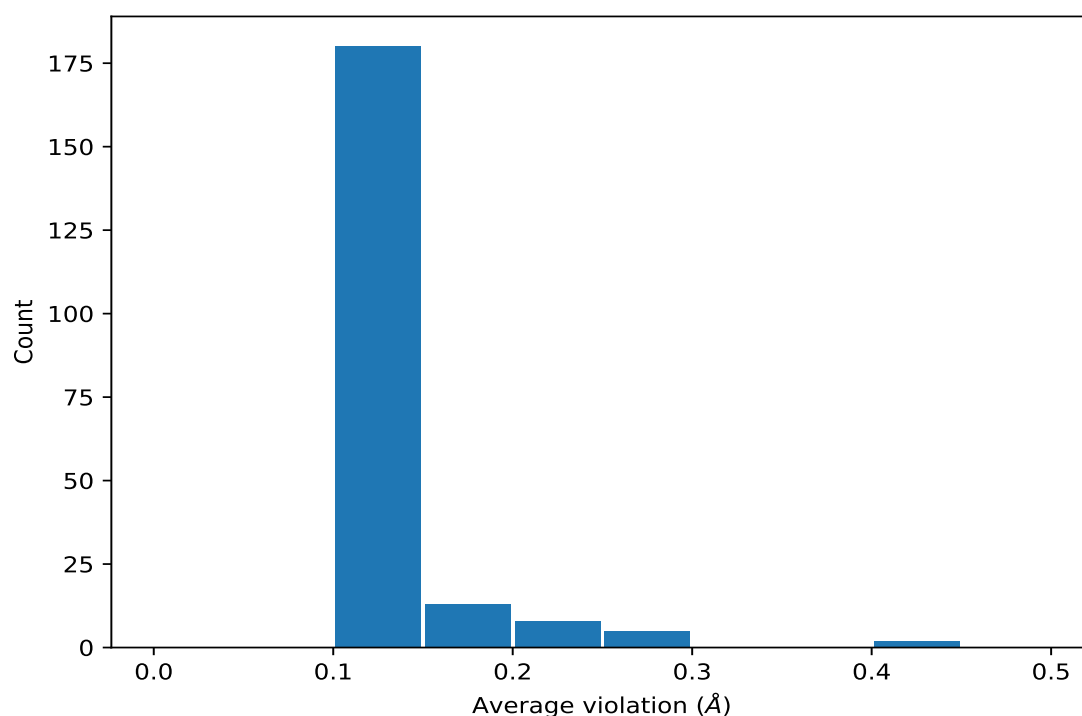


## 9.4 Most violated distance restraints in the ensemble [i](#)

### 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) |
|---------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,960) | 1:69:A:HIS:HB2 | 1:79:A:LEU:HA   | 20                  | 0.21     | 0.05                | 0.19       |
| (1,959) | 1:69:A:HIS:HB2 | 1:79:A:LEU:H    | 20                  | 0.17     | 0.04                | 0.18       |
| (2,61)  | 1:73:A:ILE:O   | 1:77:A:VAL:N    | 20                  | 0.14     | 0.0                 | 0.14       |
| (2,69)  | 1:77:A:VAL:O   | 1:81:A:GLU:N    | 20                  | 0.13     | 0.01                | 0.13       |
| (1,985) | 1:70:A:PHE:HB2 | 1:75:A:SER:HB2  | 20                  | 0.12     | 0.01                | 0.12       |
| (2,14)  | 1:10:A:GLN:O   | 1:14:A:ASP:N    | 20                  | 0.12     | 0.0                 | 0.12       |
| (1,647) | 1:45:A:LEU:HA  | 1:49:A:LEU:HA   | 19                  | 0.14     | 0.02                | 0.14       |
| (1,387) | 1:18:A:LEU:HB2 | 1:21:A:ILE:HG12 | 19                  | 0.13     | 0.02                | 0.12       |
| (1,14)  | 1:4:A:LEU:HB2  | 1:8:A:LEU:HB2   | 19                  | 0.11     | 0.01                | 0.11       |
| (1,939) | 1:66:A:THR:H   | 1:68:A:GLN:H    | 19                  | 0.11     | 0.0                 | 0.11       |
| (2,1)   | 1:4:A:LEU:O    | 1:8:A:LEU:N     | 19                  | 0.11     | 0.0                 | 0.11       |
| (1,389) | 1:18:A:LEU:HG  | 1:37:A:LEU:HB3  | 18                  | 0.27     | 0.04                | 0.26       |
| (1,337) | 1:15:A:VAL:HB  | 1:51:A:LEU:HG   | 18                  | 0.14     | 0.02                | 0.14       |
| (1,688) | 1:48:A:GLY:HA2 | 1:59:A:LEU:HB3  | 18                  | 0.13     | 0.03                | 0.12       |
| (1,961) | 1:69:A:HIS:H   | 1:75:A:SER:HB2  | 18                  | 0.12     | 0.01                | 0.12       |
| (1,917) | 1:65:A:GLU:HA  | 1:68:A:GLN:HA   | 18                  | 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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1078) | 1:75:A:SER:HB2  | 1:79:A:LEU:H    | 18                  | 0.12     | 0.01                | 0.12       |
| (1,18)   | 1:4:A:LEU:HA    | 1:8:A:LEU:HA    | 18                  | 0.12     | 0.01                | 0.11       |
| (1,225)  | 1:10:A:GLN:HA   | 1:13:A:ILE:HA   | 18                  | 0.11     | 0.01                | 0.11       |
| (1,937)  | 1:66:A:THR:H    | 1:68:A:GLN:HG3  | 18                  | 0.11     | 0.0                 | 0.11       |
| (1,360)  | 1:16:A:LEU:HB2  | 1:37:A:LEU:HG   | 17                  | 0.17     | 0.06                | 0.15       |
| (1,1169) | 1:80:A:VAL:HB   | 1:84:A:GLN:HG2  | 17                  | 0.15     | 0.02                | 0.15       |
| (1,66)   | 1:5:A:ALA:HA    | 1:73:A:ILE:HG13 | 17                  | 0.14     | 0.02                | 0.14       |
| (1,13)   | 1:4:A:LEU:HG    | 1:8:A:LEU:HA    | 17                  | 0.14     | 0.02                | 0.13       |
| (1,689)  | 1:48:A:GLY:HA3  | 1:52:A:LYS:HB2  | 17                  | 0.13     | 0.02                | 0.13       |
| (1,1091) | 1:76:A:LEU:HG   | 1:79:A:LEU:HB2  | 17                  | 0.13     | 0.02                | 0.12       |
| (1,15)   | 1:4:A:LEU:HG    | 1:7:A:GLU:HB2   | 17                  | 0.13     | 0.02                | 0.13       |
| (1,16)   | 1:4:A:LEU:HB2   | 1:77:A:VAL:HB   | 17                  | 0.12     | 0.02                | 0.12       |
| (1,758)  | 1:52:A:LYS:HG3  | 1:57:A:ILE:H    | 17                  | 0.12     | 0.01                | 0.12       |
| (1,112)  | 1:7:A:GLU:HB3   | 1:10:A:GLN:HB2  | 17                  | 0.12     | 0.01                | 0.11       |
| (1,263)  | 1:11:A:MET:HB3  | 1:15:A:VAL:H    | 17                  | 0.11     | 0.01                | 0.11       |
| (1,1032) | 1:73:A:ILE:H    | 1:76:A:LEU:HG   | 17                  | 0.11     | 0.01                | 0.11       |
| (1,723)  | 1:50:A:ALA:H    | 1:51:A:LEU:HA   | 17                  | 0.11     | 0.0                 | 0.11       |
| (1,897)  | 1:64:A:ASP:H    | 1:68:A:GLN:H    | 17                  | 0.11     | 0.01                | 0.11       |
| (1,736)  | 1:51:A:LEU:HB3  | 1:59:A:LEU:HG   | 16                  | 0.15     | 0.03                | 0.15       |
| (1,760)  | 1:52:A:LYS:HA   | 1:56:A:ASN:HB2  | 16                  | 0.15     | 0.03                | 0.15       |
| (1,19)   | 1:4:A:LEU:HG    | 1:81:A:GLU:HA   | 16                  | 0.14     | 0.02                | 0.14       |
| (1,892)  | 1:63:A:SER:HA   | 1:67:A:LYS:HG2  | 16                  | 0.13     | 0.04                | 0.12       |
| (1,986)  | 1:70:A:PHE:HB3  | 1:75:A:SER:HB2  | 16                  | 0.13     | 0.01                | 0.13       |
| (1,12)   | 1:4:A:LEU:HA    | 1:7:A:GLU:HA    | 16                  | 0.12     | 0.01                | 0.12       |
| (1,125)  | 1:8:A:LEU:HB3   | 1:77:A:VAL:HA   | 16                  | 0.12     | 0.01                | 0.12       |
| (1,1157) | 1:79:A:LEU:H    | 1:81:A:GLU:H    | 16                  | 0.12     | 0.01                | 0.12       |
| (1,27)   | 1:4:A:LEU:HB2   | 1:84:A:GLN:HG3  | 16                  | 0.12     | 0.01                | 0.12       |
| (1,673)  | 1:47:A:LEU:HB3  | 1:51:A:LEU:HG   | 16                  | 0.12     | 0.01                | 0.12       |
| (1,223)  | 1:10:A:GLN:HB2  | 1:22:A:THR:HB   | 16                  | 0.11     | 0.01                | 0.11       |
| (1,942)  | 1:66:A:THR:HB   | 1:68:A:GLN:H    | 16                  | 0.11     | 0.01                | 0.11       |
| (1,133)  | 1:8:A:LEU:HB2   | 1:12:A:ILE:HG13 | 16                  | 0.11     | 0.01                | 0.11       |
| (1,226)  | 1:10:A:GLN:HB3  | 1:14:A:ASP:H    | 16                  | 0.1      | 0.0                 | 0.1        |
| (1,737)  | 1:51:A:LEU:HA   | 1:57:A:ILE:H    | 15                  | 0.15     | 0.04                | 0.15       |
| (1,796)  | 1:55:A:TYR:HB2  | 1:83:A:GLN:HB3  | 15                  | 0.13     | 0.05                | 0.12       |
| (1,414)  | 1:21:A:ILE:HG13 | 1:25:A:ASP:HB2  | 15                  | 0.13     | 0.03                | 0.12       |
| (1,128)  | 1:8:A:LEU:HA    | 1:76:A:LEU:HB3  | 15                  | 0.13     | 0.01                | 0.13       |
| (1,795)  | 1:55:A:TYR:HB3  | 1:57:A:ILE:HA   | 15                  | 0.12     | 0.02                | 0.12       |
| (1,1158) | 1:79:A:LEU:HB3  | 1:82:A:ALA:H    | 15                  | 0.12     | 0.01                | 0.12       |
| (1,227)  | 1:10:A:GLN:HG2  | 1:14:A:ASP:HA   | 15                  | 0.12     | 0.01                | 0.11       |
| (1,1033) | 1:73:A:ILE:HA   | 1:77:A:VAL:HA   | 15                  | 0.11     | 0.01                | 0.11       |
| (1,184)  | 1:9:A:LYS:HB2   | 1:13:A:ILE:HG13 | 15                  | 0.11     | 0.01                | 0.11       |
| (1,143)  | 1:8:A:LEU:HA    | 1:12:A:ILE:HA   | 15                  | 0.11     | 0.01                | 0.11       |

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| Key      | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,71)   | 1:78:A:ALA:O   | 1:82:A:ALA:H    | 15                  | 0.11     | 0.01                | 0.11       |
| (1,1198) | 1:81:A:GLU:HA  | 1:83:A:GLN:HG2  | 14                  | 0.3      | 0.08                | 0.34       |
| (1,1079) | 1:75:A:SER:HA  | 1:79:A:LEU:HB2  | 14                  | 0.16     | 0.02                | 0.16       |
| (1,406)  | 1:19:A:GLU:HB3 | 1:21:A:ILE:H    | 14                  | 0.16     | 0.04                | 0.15       |
| (1,2)    | 1:2:A:SER:H    | 1:4:A:LEU:HB3   | 14                  | 0.14     | 0.02                | 0.14       |
| (1,857)  | 1:60:A:ASN:HB2 | 1:66:A:THR:HA   | 14                  | 0.14     | 0.03                | 0.12       |
| (1,600)  | 1:41:A:SER:HA  | 1:45:A:LEU:H    | 14                  | 0.13     | 0.02                | 0.13       |
| (1,891)  | 1:63:A:SER:H   | 1:65:A:GLU:H    | 14                  | 0.13     | 0.01                | 0.13       |
| (1,962)  | 1:69:A:HIS:HB2 | 1:76:A:LEU:HG   | 14                  | 0.13     | 0.01                | 0.12       |
| (1,886)  | 1:62:A:GLU:HA  | 1:67:A:LYS:HG2  | 14                  | 0.13     | 0.02                | 0.12       |
| (1,722)  | 1:50:A:ALA:HA  | 1:52:A:LYS:HB3  | 14                  | 0.12     | 0.02                | 0.12       |
| (1,257)  | 1:11:A:MET:HA  | 1:15:A:VAL:HA   | 14                  | 0.12     | 0.01                | 0.12       |
| (1,631)  | 1:44:A:ALA:HA  | 1:47:A:LEU:HG   | 14                  | 0.11     | 0.01                | 0.11       |
| (1,1145) | 1:78:A:ALA:H   | 1:80:A:VAL:H    | 14                  | 0.11     | 0.01                | 0.11       |
| (1,1064) | 1:74:A:GLN:H   | 1:77:A:VAL:HB   | 14                  | 0.11     | 0.01                | 0.11       |
| (1,186)  | 1:9:A:LYS:H    | 1:11:A:MET:HB2  | 14                  | 0.11     | 0.01                | 0.11       |
| (1,183)  | 1:9:A:LYS:HB2  | 1:13:A:ILE:H    | 14                  | 0.11     | 0.01                | 0.11       |
| (1,691)  | 1:48:A:GLY:HA3 | 1:51:A:LEU:HB3  | 14                  | 0.11     | 0.01                | 0.11       |
| (1,127)  | 1:8:A:LEU:HA   | 1:12:A:ILE:HB   | 14                  | 0.11     | 0.01                | 0.11       |
| (1,23)   | 1:4:A:LEU:HA   | 1:8:A:LEU:HB2   | 14                  | 0.11     | 0.01                | 0.11       |
| (1,1149) | 1:78:A:ALA:H   | 1:82:A:ALA:H    | 14                  | 0.11     | 0.01                | 0.11       |
| (1,258)  | 1:11:A:MET:HB2 | 1:15:A:VAL:HB   | 13                  | 0.12     | 0.02                | 0.11       |
| (1,628)  | 1:44:A:ALA:HA  | 1:48:A:GLY:HA3  | 13                  | 0.12     | 0.01                | 0.12       |
| (1,858)  | 1:60:A:ASN:HA  | 1:66:A:THR:H    | 13                  | 0.12     | 0.02                | 0.13       |
| (1,479)  | 1:29:A:GLU:HA  | 1:72:A:SER:H    | 13                  | 0.12     | 0.02                | 0.12       |
| (1,707)  | 1:49:A:LEU:HA  | 1:53:A:LYS:H    | 13                  | 0.12     | 0.02                | 0.12       |
| (1,687)  | 1:48:A:GLY:HA2 | 1:59:A:LEU:HB2  | 13                  | 0.12     | 0.02                | 0.12       |
| (1,692)  | 1:48:A:GLY:HA2 | 1:51:A:LEU:HA   | 13                  | 0.12     | 0.01                | 0.12       |
| (1,131)  | 1:8:A:LEU:HA   | 1:12:A:ILE:HG12 | 13                  | 0.11     | 0.01                | 0.11       |
| (1,111)  | 1:7:A:GLU:H    | 1:10:A:GLN:HB2  | 13                  | 0.11     | 0.01                | 0.11       |
| (1,185)  | 1:9:A:LYS:HB3  | 1:12:A:ILE:H    | 13                  | 0.11     | 0.01                | 0.11       |
| (1,938)  | 1:66:A:THR:H   | 1:69:A:HIS:H    | 13                  | 0.11     | 0.01                | 0.11       |
| (1,1113) | 1:77:A:VAL:HB  | 1:79:A:LEU:H    | 13                  | 0.11     | 0.01                | 0.11       |
| (1,228)  | 1:10:A:GLN:HG3 | 1:22:A:THR:HA   | 13                  | 0.11     | 0.01                | 0.11       |
| (2,8)    | 1:7:A:GLU:O    | 1:11:A:MET:N    | 13                  | 0.11     | 0.01                | 0.11       |
| (1,224)  | 1:10:A:GLN:H   | 1:12:A:ILE:HA   | 13                  | 0.1      | 0.0                 | 0.1        |
| (1,789)  | 1:54:A:ARG:H   | 1:55:A:TYR:HA   | 12                  | 0.16     | 0.08                | 0.12       |
| (1,651)  | 1:45:A:LEU:HA  | 1:48:A:GLY:HA2  | 12                  | 0.13     | 0.03                | 0.12       |
| (1,877)  | 1:61:A:ALA:HA  | 1:66:A:THR:H    | 12                  | 0.13     | 0.02                | 0.12       |
| (1,26)   | 1:4:A:LEU:HB3  | 1:81:A:GLU:HA   | 12                  | 0.13     | 0.02                | 0.12       |
| (1,308)  | 1:13:A:ILE:HA  | 1:18:A:LEU:HA   | 12                  | 0.12     | 0.02                | 0.12       |
| (1,7)    | 1:3:A:ASN:H    | 1:84:A:GLN:HE22 | 12                  | 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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,674)  | 1:47:A:LEU:HG   | 1:51:A:LEU:HB3  | 12                  | 0.12     | 0.02                | 0.12       |
| (1,22)   | 1:4:A:LEU:HB2   | 1:77:A:VAL:HA   | 12                  | 0.12     | 0.01                | 0.12       |
| (1,616)  | 1:43:A:ASP:HA   | 1:46:A:GLU:HA   | 12                  | 0.11     | 0.01                | 0.11       |
| (1,629)  | 1:44:A:ALA:H    | 1:47:A:LEU:HB2  | 12                  | 0.11     | 0.01                | 0.11       |
| (1,1080) | 1:75:A:SER:HB3  | 1:79:A:LEU:HG   | 12                  | 0.11     | 0.01                | 0.11       |
| (1,187)  | 1:9:A:LYS:H     | 1:12:A:ILE:HB   | 12                  | 0.11     | 0.01                | 0.1        |
| (1,829)  | 1:57:A:ILE:HA   | 1:80:A:VAL:HA   | 11                  | 0.2      | 0.07                | 0.22       |
| (1,1175) | 1:80:A:VAL:HA   | 1:84:A:GLN:HG2  | 11                  | 0.15     | 0.03                | 0.14       |
| (1,1094) | 1:76:A:LEU:HB3  | 1:79:A:LEU:H    | 11                  | 0.13     | 0.03                | 0.14       |
| (1,618)  | 1:43:A:ASP:HB3  | 1:46:A:GLU:H    | 11                  | 0.13     | 0.02                | 0.12       |
| (1,362)  | 1:16:A:LEU:HG   | 1:43:A:ASP:HB2  | 11                  | 0.12     | 0.03                | 0.12       |
| (1,1156) | 1:79:A:LEU:HB2  | 1:82:A:ALA:H    | 11                  | 0.12     | 0.01                | 0.11       |
| (1,231)  | 1:10:A:GLN:HA   | 1:12:A:ILE:HB   | 11                  | 0.12     | 0.01                | 0.11       |
| (1,232)  | 1:10:A:GLN:HG3  | 1:23:A:ILE:HG13 | 11                  | 0.11     | 0.01                | 0.11       |
| (1,136)  | 1:8:A:LEU:HB3   | 1:12:A:ILE:HA   | 11                  | 0.11     | 0.01                | 0.11       |
| (1,676)  | 1:47:A:LEU:HA   | 1:49:A:LEU:H    | 11                  | 0.11     | 0.01                | 0.11       |
| (1,834)  | 1:57:A:ILE:HB   | 1:80:A:VAL:HA   | 10                  | 0.42     | 0.03                | 0.43       |
| (1,709)  | 1:49:A:LEU:HA   | 1:59:A:LEU:HG   | 10                  | 0.24     | 0.21                | 0.13       |
| (1,1170) | 1:80:A:VAL:HB   | 1:82:A:ALA:H    | 10                  | 0.16     | 0.02                | 0.16       |
| (1,759)  | 1:52:A:LYS:HG2  | 1:58:A:HIS:H    | 10                  | 0.15     | 0.01                | 0.16       |
| (1,710)  | 1:49:A:LEU:HA   | 1:52:A:LYS:HG2  | 10                  | 0.13     | 0.01                | 0.13       |
| (1,68)   | 1:5:A:ALA:HA    | 1:9:A:LYS:HB2   | 10                  | 0.13     | 0.03                | 0.12       |
| (1,1035) | 1:73:A:ILE:HG12 | 1:76:A:LEU:HB2  | 10                  | 0.13     | 0.02                | 0.12       |
| (1,182)  | 1:9:A:LYS:HA    | 1:13:A:ILE:HB   | 10                  | 0.12     | 0.02                | 0.12       |
| (1,708)  | 1:49:A:LEU:HB2  | 1:52:A:LYS:H    | 10                  | 0.12     | 0.01                | 0.12       |
| (1,940)  | 1:66:A:THR:H    | 1:70:A:PHE:H    | 10                  | 0.12     | 0.02                | 0.11       |
| (1,137)  | 1:8:A:LEU:HA    | 1:76:A:LEU:HB2  | 10                  | 0.11     | 0.01                | 0.11       |
| (1,1034) | 1:73:A:ILE:HB   | 1:77:A:VAL:HB   | 10                  | 0.11     | 0.0                 | 0.11       |
| (1,113)  | 1:7:A:GLU:HA    | 1:11:A:MET:HB3  | 10                  | 0.11     | 0.01                | 0.11       |
| (1,142)  | 1:8:A:LEU:HA    | 1:11:A:MET:HA   | 10                  | 0.11     | 0.01                | 0.11       |
| (1,138)  | 1:8:A:LEU:HB2   | 1:11:A:MET:H    | 10                  | 0.1      | 0.0                 | 0.1        |
| (1,230)  | 1:10:A:GLN:HB2  | 1:14:A:ASP:H    | 10                  | 0.1      | 0.0                 | 0.1        |
| (1,289)  | 1:12:A:ILE:HG13 | 1:15:A:VAL:H    | 10                  | 0.1      | 0.0                 | 0.1        |
| (1,738)  | 1:51:A:LEU:HA   | 1:57:A:ILE:HB   | 9                   | 0.25     | 0.06                | 0.24       |
| (1,649)  | 1:45:A:LEU:HB2  | 1:49:A:LEU:HB3  | 9                   | 0.19     | 0.01                | 0.19       |
| (1,761)  | 1:52:A:LYS:HA   | 1:56:A:ASN:HB3  | 9                   | 0.17     | 0.04                | 0.18       |
| (1,739)  | 1:51:A:LEU:HB3  | 1:54:A:ARG:HB3  | 9                   | 0.16     | 0.03                | 0.15       |
| (1,832)  | 1:57:A:ILE:HB   | 1:59:A:LEU:HG   | 9                   | 0.14     | 0.01                | 0.14       |
| (1,794)  | 1:55:A:TYR:HB2  | 1:84:A:GLN:HG2  | 9                   | 0.14     | 0.03                | 0.15       |
| (1,648)  | 1:45:A:LEU:HB2  | 1:49:A:LEU:H    | 9                   | 0.13     | 0.01                | 0.13       |
| (1,572)  | 1:39:A:LEU:HA   | 1:43:A:ASP:H    | 9                   | 0.12     | 0.02                | 0.12       |
| (1,1217) | 1:83:A:GLN:H    | 1:85:A:LYS:H    | 9                   | 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) |
|----------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,1168) | 1:80:A:VAL:HA   | 1:83:A:GLN:HA  | 9                   | 0.12     | 0.01                | 0.12       |
| (1,675)  | 1:47:A:LEU:HA   | 1:51:A:LEU:HA  | 9                   | 0.12     | 0.01                | 0.12       |
| (1,286)  | 1:12:A:ILE:H    | 1:14:A:ASP:H   | 9                   | 0.1      | 0.0                 | 0.1        |
| (1,229)  | 1:10:A:GLN:H    | 1:14:A:ASP:HB3 | 9                   | 0.1      | 0.0                 | 0.1        |
| (1,1159) | 1:79:A:LEU:HA   | 1:83:A:GLN:HB3 | 8                   | 0.17     | 0.02                | 0.16       |
| (1,535)  | 1:33:A:PHE:HA   | 1:39:A:LEU:HB3 | 8                   | 0.15     | 0.04                | 0.15       |
| (1,693)  | 1:48:A:GLY:HA3  | 1:51:A:LEU:HG  | 8                   | 0.12     | 0.01                | 0.12       |
| (1,800)  | 1:55:A:TYR:HB3  | 1:80:A:VAL:HA  | 8                   | 0.12     | 0.02                | 0.12       |
| (1,517)  | 1:32:A:LEU:HB2  | 1:39:A:LEU:H   | 8                   | 0.12     | 0.02                | 0.12       |
| (1,1118) | 1:77:A:VAL:HB   | 1:81:A:GLU:H   | 8                   | 0.12     | 0.01                | 0.12       |
| (1,724)  | 1:50:A:ALA:H    | 1:52:A:LYS:HB3 | 8                   | 0.12     | 0.02                | 0.11       |
| (1,903)  | 1:64:A:ASP:H    | 1:67:A:LYS:H   | 8                   | 0.11     | 0.01                | 0.11       |
| (1,388)  | 1:18:A:LEU:HB3  | 1:21:A:ILE:HA  | 8                   | 0.11     | 0.0                 | 0.11       |
| (1,988)  | 1:70:A:PHE:HB2  | 1:76:A:LEU:HG  | 8                   | 0.1      | 0.0                 | 0.1        |
| (1,951)  | 1:67:A:LYS:HA   | 1:71:A:LYS:H   | 7                   | 0.13     | 0.04                | 0.11       |
| (1,784)  | 1:53:A:LYS:HA   | 1:55:A:TYR:H   | 7                   | 0.13     | 0.02                | 0.12       |
| (1,833)  | 1:57:A:ILE:HA   | 1:59:A:LEU:H   | 7                   | 0.12     | 0.01                | 0.12       |
| (1,480)  | 1:29:A:GLU:H    | 1:74:A:GLN:HB3 | 7                   | 0.12     | 0.02                | 0.12       |
| (1,190)  | 1:9:A:LYS:HA    | 1:73:A:ILE:HB  | 7                   | 0.11     | 0.01                | 0.11       |
| (1,1039) | 1:73:A:ILE:HB   | 1:76:A:LEU:HG  | 7                   | 0.11     | 0.01                | 0.11       |
| (1,1213) | 1:82:A:ALA:HA   | 1:84:A:GLN:H   | 7                   | 0.11     | 0.01                | 0.11       |
| (1,941)  | 1:66:A:THR:H    | 1:68:A:GLN:HG2 | 7                   | 0.11     | 0.01                | 0.11       |
| (1,365)  | 1:16:A:LEU:HG   | 1:39:A:LEU:HB3 | 6                   | 0.42     | 0.16                | 0.35       |
| (1,652)  | 1:45:A:LEU:HA   | 1:49:A:LEU:HB3 | 6                   | 0.12     | 0.01                | 0.12       |
| (1,571)  | 1:39:A:LEU:HB2  | 1:43:A:ASP:H   | 6                   | 0.12     | 0.01                | 0.12       |
| (2,51)   | 1:63:A:SER:O    | 1:67:A:LYS:H   | 6                   | 0.11     | 0.01                | 0.11       |
| (1,963)  | 1:69:A:HIS:HA   | 1:76:A:LEU:HA  | 6                   | 0.11     | 0.01                | 0.11       |
| (1,357)  | 1:16:A:LEU:HB2  | 1:18:A:LEU:HA  | 6                   | 0.11     | 0.01                | 0.11       |
| (1,943)  | 1:66:A:THR:HB   | 1:69:A:HIS:H   | 6                   | 0.11     | 0.0                 | 0.11       |
| (1,665)  | 1:46:A:GLU:H    | 1:47:A:LEU:HB2 | 6                   | 0.1      | 0.0                 | 0.11       |
| (1,364)  | 1:16:A:LEU:HD11 | 1:43:A:ASP:HA  | 5                   | 0.18     | 0.01                | 0.18       |
| (1,364)  | 1:16:A:LEU:HD12 | 1:43:A:ASP:HA  | 5                   | 0.18     | 0.01                | 0.18       |
| (1,364)  | 1:16:A:LEU:HD13 | 1:43:A:ASP:HA  | 5                   | 0.18     | 0.01                | 0.18       |
| (2,49)   | 1:52:A:LYS:O    | 1:56:A:ASN:N   | 5                   | 0.12     | 0.01                | 0.12       |
| (1,1121) | 1:77:A:VAL:HA   | 1:80:A:VAL:HA  | 5                   | 0.11     | 0.01                | 0.11       |
| (1,191)  | 1:9:A:LYS:HA    | 1:13:A:ILE:HA  | 5                   | 0.1      | 0.0                 | 0.1        |
| (1,727)  | 1:50:A:ALA:HA   | 1:54:A:ARG:HG2 | 4                   | 0.3      | 0.03                | 0.3        |
| (1,727)  | 1:50:A:ALA:HA   | 1:54:A:ARG:HG3 | 4                   | 0.3      | 0.03                | 0.3        |
| (1,859)  | 1:60:A:ASN:HB2  | 1:63:A:SER:HA  | 4                   | 0.14     | 0.05                | 0.12       |
| (1,1227) | 1:84:A:GLN:H    | 1:85:A:LYS:HB2 | 4                   | 0.11     | 0.01                | 0.11       |
| (1,95)   | 1:6:A:ASP:HB2   | 1:8:A:LEU:H    | 4                   | 0.11     | 0.01                | 0.1        |
| (2,40)   | 1:47:A:LEU:O    | 1:51:A:LEU:N   | 4                   | 0.11     | 0.01                | 0.1        |

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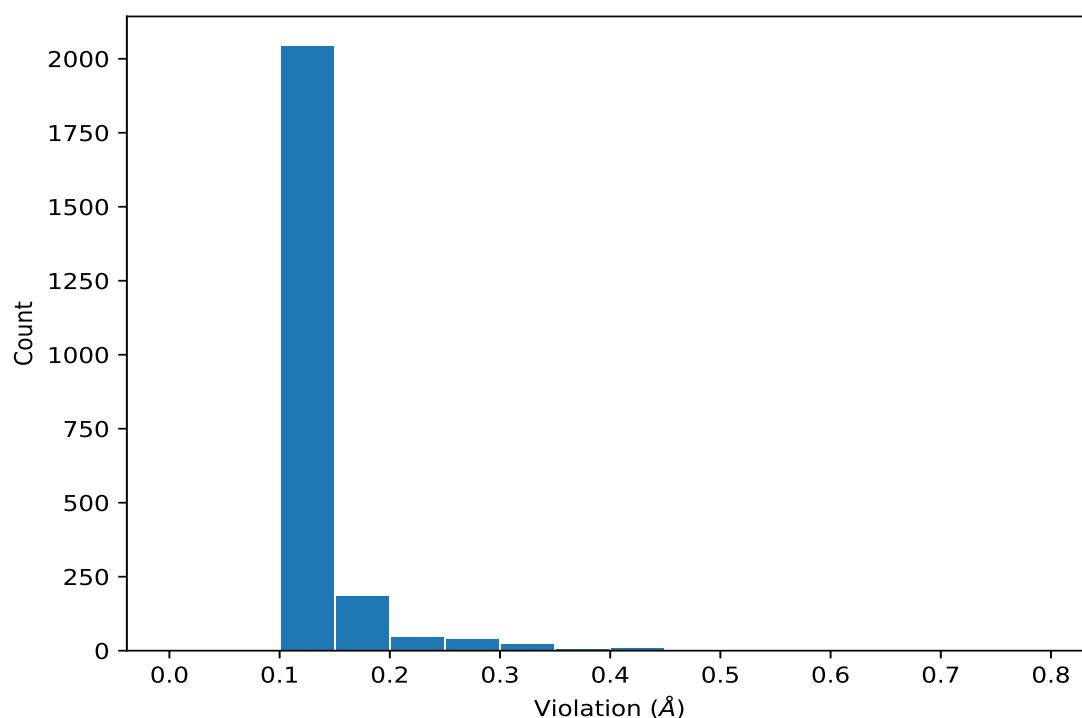
| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,741)  | 1:51:A:LEU:H    | 1:52:A:LYS:HA   | 4                   | 0.1      | 0.0                 | 0.11       |
| (1,505)  | 1:31:A:PRO:HB3  | 1:34:A:GLY:HA2  | 3                   | 0.13     | 0.02                | 0.13       |
| (1,559)  | 1:37:A:LEU:HB2  | 1:39:A:LEU:HA   | 3                   | 0.13     | 0.01                | 0.12       |
| (1,503)  | 1:31:A:PRO:HB2  | 1:35:A:GLU:HB3  | 3                   | 0.12     | 0.02                | 0.12       |
| (1,545)  | 1:33:A:PHE:HE1  | 1:40:A:ASP:H    | 3                   | 0.12     | 0.01                | 0.12       |
| (2,9)    | 1:8:A:LEU:O     | 1:12:A:ILE:N    | 3                   | 0.11     | 0.0                 | 0.11       |
| (2,15)   | 1:11:A:MET:O    | 1:15:A:VAL:N    | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,601)  | 1:41:A:SER:HA   | 1:44:A:ALA:HA   | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,1221) | 1:83:A:GLN:HB3  | 1:84:A:GLN:H    | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,765)  | 1:52:A:LYS:HG2  | 1:57:A:ILE:HA   | 2                   | 0.22     | 0.01                | 0.22       |
| (1,711)  | 1:49:A:LEU:HA   | 1:53:A:LYS:HG2  | 2                   | 0.21     | 0.07                | 0.21       |
| (1,464)  | 1:28:A:THR:HG23 | 1:74:A:GLN:HA   | 2                   | 0.21     | 0.1                 | 0.21       |
| (1,830)  | 1:57:A:ILE:HG12 | 1:83:A:GLN:HB2  | 2                   | 0.2      | 0.0                 | 0.2        |
| (1,830)  | 1:57:A:ILE:HG13 | 1:83:A:GLN:HB2  | 2                   | 0.2      | 0.0                 | 0.2        |
| (1,797)  | 1:55:A:TYR:HB2  | 1:57:A:ILE:HG12 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,797)  | 1:55:A:TYR:HB2  | 1:57:A:ILE:HG13 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,850)  | 1:59:A:LEU:HB2  | 1:61:A:ALA:HA   | 2                   | 0.13     | 0.01                | 0.13       |
| (1,70)   | 1:5:A:ALA:H     | 1:77:A:VAL:HA   | 2                   | 0.12     | 0.01                | 0.12       |
| (1,193)  | 1:9:A:LYS:HA    | 1:26:A:ILE:HB   | 2                   | 0.12     | 0.01                | 0.12       |
| (1,536)  | 1:33:A:PHE:HE1  | 1:39:A:LEU:H    | 2                   | 0.12     | 0.01                | 0.12       |
| (1,740)  | 1:51:A:LEU:H    | 1:52:A:LYS:HB3  | 2                   | 0.11     | 0.01                | 0.11       |
| (1,763)  | 1:52:A:LYS:HA   | 1:59:A:LEU:H    | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,55)   | 1:65:A:GLU:O    | 1:69:A:HIS:H    | 2                   | 0.1      | 0.0                 | 0.1        |
| (2,73)   | 1:79:A:LEU:O    | 1:83:A:GLN:H    | 2                   | 0.1      | 0.0                 | 0.1        |

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

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

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

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



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

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

| Key      | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|----------|---------------|----------------|----------|---------------|
| (1,365)  | 1:16:A:LEU:HG | 1:39:A:LEU:HB3 | 5        | 0.78          |
| (1,709)  | 1:49:A:LEU:HA | 1:59:A:LEU:HG  | 9        | 0.68          |
| (1,709)  | 1:49:A:LEU:HA | 1:59:A:LEU:HG  | 17       | 0.63          |
| (1,834)  | 1:57:A:ILE:HB | 1:80:A:VAL:HA  | 7        | 0.45          |
| (1,834)  | 1:57:A:ILE:HB | 1:80:A:VAL:HA  | 15       | 0.45          |
| (1,834)  | 1:57:A:ILE:HB | 1:80:A:VAL:HA  | 20       | 0.45          |
| (1,834)  | 1:57:A:ILE:HB | 1:80:A:VAL:HA  | 3        | 0.44          |
| (1,834)  | 1:57:A:ILE:HB | 1:80:A:VAL:HA  | 4        | 0.43          |
| (1,834)  | 1:57:A:ILE:HB | 1:80:A:VAL:HA  | 14       | 0.43          |
| (1,834)  | 1:57:A:ILE:HB | 1:80:A:VAL:HA  | 19       | 0.42          |
| (1,834)  | 1:57:A:ILE:HB | 1:80:A:VAL:HA  | 1        | 0.41          |
| (1,834)  | 1:57:A:ILE:HB | 1:80:A:VAL:HA  | 9        | 0.41          |
| (1,1198) | 1:81:A:GLU:HA | 1:83:A:GLN:HG2 | 17       | 0.4           |
| (1,1198) | 1:81:A:GLU:HA | 1:83:A:GLN:HG2 | 14       | 0.37          |
| (1,365)  | 1:16:A:LEU:HG | 1:39:A:LEU:HB3 | 14       | 0.37          |
| (1,1198) | 1:81:A:GLU:HA | 1:83:A:GLN:HG2 | 9        | 0.36          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1198) | 1:81:A:GLU:HA   | 1:83:A:GLN:HG2 | 15       | 0.36          |
| (1,1198) | 1:81:A:GLU:HA   | 1:83:A:GLN:HG2 | 19       | 0.36          |
| (1,834)  | 1:57:A:ILE:HB   | 1:80:A:VAL:HA  | 17       | 0.36          |
| (1,1198) | 1:81:A:GLU:HA   | 1:83:A:GLN:HG2 | 7        | 0.35          |
| (1,365)  | 1:16:A:LEU:HG   | 1:39:A:LEU:HB3 | 6        | 0.35          |
| (1,365)  | 1:16:A:LEU:HG   | 1:39:A:LEU:HB3 | 16       | 0.35          |
| (1,1198) | 1:81:A:GLU:HA   | 1:83:A:GLN:HG2 | 1        | 0.34          |
| (1,1198) | 1:81:A:GLU:HA   | 1:83:A:GLN:HG2 | 3        | 0.34          |
| (1,727)  | 1:50:A:ALA:HA   | 1:54:A:ARG:HG2 | 10       | 0.34          |
| (1,727)  | 1:50:A:ALA:HA   | 1:54:A:ARG:HG3 | 10       | 0.34          |
| (1,365)  | 1:16:A:LEU:HG   | 1:39:A:LEU:HB3 | 11       | 0.34          |
| (1,365)  | 1:16:A:LEU:HG   | 1:39:A:LEU:HB3 | 15       | 0.34          |
| (1,360)  | 1:16:A:LEU:HB2  | 1:37:A:LEU:HG  | 5        | 0.34          |
| (1,738)  | 1:51:A:LEU:HA   | 1:57:A:ILE:HB  | 12       | 0.33          |
| (1,389)  | 1:18:A:LEU:HG   | 1:37:A:LEU:HB3 | 2        | 0.33          |
| (1,1198) | 1:81:A:GLU:HA   | 1:83:A:GLN:HG2 | 20       | 0.32          |
| (1,738)  | 1:51:A:LEU:HA   | 1:57:A:ILE:HB  | 2        | 0.32          |
| (1,389)  | 1:18:A:LEU:HG   | 1:37:A:LEU:HB3 | 9        | 0.32          |
| (1,389)  | 1:18:A:LEU:HG   | 1:37:A:LEU:HB3 | 19       | 0.32          |
| (1,796)  | 1:55:A:TYR:HB2  | 1:83:A:GLN:HB3 | 4        | 0.31          |
| (1,738)  | 1:51:A:LEU:HA   | 1:57:A:ILE:HB  | 11       | 0.31          |
| (1,727)  | 1:50:A:ALA:HA   | 1:54:A:ARG:HG2 | 17       | 0.31          |
| (1,727)  | 1:50:A:ALA:HA   | 1:54:A:ARG:HG3 | 17       | 0.31          |
| (1,464)  | 1:28:A:THR:HG23 | 1:74:A:GLN:HA  | 19       | 0.31          |
| (1,960)  | 1:69:A:HIS:HB2  | 1:79:A:LEU:HA  | 5        | 0.3           |
| (1,960)  | 1:69:A:HIS:HB2  | 1:79:A:LEU:HA  | 12       | 0.3           |
| (1,389)  | 1:18:A:LEU:HG   | 1:37:A:LEU:HB3 | 5        | 0.3           |
| (1,389)  | 1:18:A:LEU:HG   | 1:37:A:LEU:HB3 | 11       | 0.3           |
| (1,389)  | 1:18:A:LEU:HG   | 1:37:A:LEU:HB3 | 13       | 0.3           |
| (1,1198) | 1:81:A:GLU:HA   | 1:83:A:GLN:HG2 | 4        | 0.29          |
| (1,829)  | 1:57:A:ILE:HA   | 1:80:A:VAL:HA  | 8        | 0.29          |
| (1,789)  | 1:54:A:ARG:H    | 1:55:A:TYR:HA  | 1        | 0.29          |
| (1,789)  | 1:54:A:ARG:H    | 1:55:A:TYR:HA  | 7        | 0.29          |
| (1,789)  | 1:54:A:ARG:H    | 1:55:A:TYR:HA  | 3        | 0.28          |
| (1,727)  | 1:50:A:ALA:HA   | 1:54:A:ARG:HG2 | 16       | 0.28          |
| (1,727)  | 1:50:A:ALA:HA   | 1:54:A:ARG:HG3 | 16       | 0.28          |
| (1,711)  | 1:49:A:LEU:HA   | 1:53:A:LYS:HG2 | 18       | 0.28          |
| (1,389)  | 1:18:A:LEU:HG   | 1:37:A:LEU:HB3 | 14       | 0.28          |
| (1,960)  | 1:69:A:HIS:HB2  | 1:79:A:LEU:HA  | 15       | 0.27          |
| (1,829)  | 1:57:A:ILE:HA   | 1:80:A:VAL:HA  | 10       | 0.27          |
| (1,829)  | 1:57:A:ILE:HA   | 1:80:A:VAL:HA  | 11       | 0.27          |
| (1,727)  | 1:50:A:ALA:HA   | 1:54:A:ARG:HG2 | 14       | 0.27          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,727)  | 1:50:A:ALA:HA  | 1:54:A:ARG:HG3 | 14       | 0.27          |
| (1,389)  | 1:18:A:LEU:HG  | 1:37:A:LEU:HB3 | 7        | 0.27          |
| (1,389)  | 1:18:A:LEU:HG  | 1:37:A:LEU:HB3 | 15       | 0.27          |
| (1,1229) | 1:84:A:GLN:H   | 1:85:A:LYS:HG3 | 5        | 0.26          |
| (1,960)  | 1:69:A:HIS:HB2 | 1:79:A:LEU:HA  | 3        | 0.26          |
| (1,960)  | 1:69:A:HIS:HB2 | 1:79:A:LEU:HA  | 7        | 0.26          |
| (1,960)  | 1:69:A:HIS:HB2 | 1:79:A:LEU:HA  | 20       | 0.26          |
| (1,892)  | 1:63:A:SER:HA  | 1:67:A:LYS:HG2 | 10       | 0.26          |
| (1,829)  | 1:57:A:ILE:HA  | 1:80:A:VAL:HA  | 2        | 0.26          |
| (1,829)  | 1:57:A:ILE:HA  | 1:80:A:VAL:HA  | 12       | 0.26          |
| (1,737)  | 1:51:A:LEU:HA  | 1:57:A:ILE:H   | 9        | 0.26          |
| (1,389)  | 1:18:A:LEU:HG  | 1:37:A:LEU:HB3 | 4        | 0.26          |
| (1,959)  | 1:69:A:HIS:HB2 | 1:79:A:LEU:H   | 12       | 0.25          |
| (1,738)  | 1:51:A:LEU:HA  | 1:57:A:ILE:HB  | 8        | 0.25          |
| (1,389)  | 1:18:A:LEU:HG  | 1:37:A:LEU:HB3 | 1        | 0.25          |
| (1,389)  | 1:18:A:LEU:HG  | 1:37:A:LEU:HB3 | 6        | 0.25          |
| (1,389)  | 1:18:A:LEU:HG  | 1:37:A:LEU:HB3 | 12       | 0.25          |
| (1,389)  | 1:18:A:LEU:HG  | 1:37:A:LEU:HB3 | 16       | 0.25          |
| (1,389)  | 1:18:A:LEU:HG  | 1:37:A:LEU:HB3 | 17       | 0.25          |
| (1,389)  | 1:18:A:LEU:HG  | 1:37:A:LEU:HB3 | 18       | 0.25          |
| (1,959)  | 1:69:A:HIS:HB2 | 1:79:A:LEU:H   | 5        | 0.24          |
| (1,738)  | 1:51:A:LEU:HA  | 1:57:A:ILE:HB  | 13       | 0.24          |
| (1,463)  | 1:28:A:THR:HG1 | 1:74:A:GLN:HG2 | 19       | 0.24          |
| (1,761)  | 1:52:A:LYS:HA  | 1:56:A:ASN:HB3 | 18       | 0.23          |
| (1,760)  | 1:52:A:LYS:HA  | 1:56:A:ASN:HB2 | 17       | 0.23          |
| (1,738)  | 1:51:A:LEU:HA  | 1:57:A:ILE:HB  | 6        | 0.23          |
| (1,389)  | 1:18:A:LEU:HG  | 1:37:A:LEU:HB3 | 8        | 0.23          |
| (1,859)  | 1:60:A:ASN:HB2 | 1:63:A:SER:HA  | 5        | 0.22          |
| (1,829)  | 1:57:A:ILE:HA  | 1:80:A:VAL:HA  | 18       | 0.22          |
| (1,765)  | 1:52:A:LYS:HG2 | 1:57:A:ILE:HA  | 17       | 0.22          |
| (1,739)  | 1:51:A:LEU:HB3 | 1:54:A:ARG:HB3 | 7        | 0.22          |
| (1,535)  | 1:33:A:PHE:HA  | 1:39:A:LEU:HB3 | 15       | 0.22          |
| (1,362)  | 1:16:A:LEU:HG  | 1:43:A:ASP:HB2 | 5        | 0.22          |
| (1,360)  | 1:16:A:LEU:HB2 | 1:37:A:LEU:HG  | 14       | 0.22          |
| (1,1198) | 1:81:A:GLU:HA  | 1:83:A:GLN:HG2 | 13       | 0.21          |
| (1,1169) | 1:80:A:VAL:HB  | 1:84:A:GLN:HG2 | 15       | 0.21          |
| (1,1079) | 1:75:A:SER:HA  | 1:79:A:LEU:HB2 | 18       | 0.21          |
| (1,960)  | 1:69:A:HIS:HB2 | 1:79:A:LEU:HA  | 11       | 0.21          |
| (1,959)  | 1:69:A:HIS:HB2 | 1:79:A:LEU:H   | 15       | 0.21          |
| (1,959)  | 1:69:A:HIS:HB2 | 1:79:A:LEU:H   | 20       | 0.21          |
| (1,918)  | 1:65:A:GLU:HG2 | 1:69:A:HIS:H   | 13       | 0.21          |
| (1,918)  | 1:65:A:GLU:HG3 | 1:69:A:HIS:H   | 13       | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,765)  | 1:52:A:LYS:HG2  | 1:57:A:ILE:HA   | 15       | 0.21          |
| (1,761)  | 1:52:A:LYS:HA   | 1:56:A:ASN:HB3  | 16       | 0.21          |
| (1,738)  | 1:51:A:LEU:HA   | 1:57:A:ILE:HB   | 5        | 0.21          |
| (1,736)  | 1:51:A:LEU:HB3  | 1:59:A:LEU:HG   | 1        | 0.21          |
| (1,406)  | 1:19:A:GLU:HB3  | 1:21:A:ILE:H    | 13       | 0.21          |
| (1,360)  | 1:16:A:LEU:HB2  | 1:37:A:LEU:HG   | 15       | 0.21          |
| (1,360)  | 1:16:A:LEU:HB2  | 1:37:A:LEU:HG   | 16       | 0.21          |
| (1,1198) | 1:81:A:GLU:HA   | 1:83:A:GLN:HG2  | 6        | 0.2           |
| (1,960)  | 1:69:A:HIS:HB2  | 1:79:A:LEU:HA   | 8        | 0.2           |
| (1,960)  | 1:69:A:HIS:HB2  | 1:79:A:LEU:HA   | 18       | 0.2           |
| (1,959)  | 1:69:A:HIS:HB2  | 1:79:A:LEU:H    | 3        | 0.2           |
| (1,951)  | 1:67:A:LYS:HA   | 1:71:A:LYS:H    | 17       | 0.2           |
| (1,830)  | 1:57:A:ILE:HG12 | 1:83:A:GLN:HB2  | 6        | 0.2           |
| (1,830)  | 1:57:A:ILE:HG13 | 1:83:A:GLN:HB2  | 6        | 0.2           |
| (1,830)  | 1:57:A:ILE:HG12 | 1:83:A:GLN:HB2  | 13       | 0.2           |
| (1,830)  | 1:57:A:ILE:HG13 | 1:83:A:GLN:HB2  | 13       | 0.2           |
| (1,794)  | 1:55:A:TYR:HB2  | 1:84:A:GLN:HG2  | 10       | 0.2           |
| (1,688)  | 1:48:A:GLY:HA2  | 1:59:A:LEU:HB3  | 3        | 0.2           |
| (1,649)  | 1:45:A:LEU:HB2  | 1:49:A:LEU:HB3  | 1        | 0.2           |
| (1,649)  | 1:45:A:LEU:HB2  | 1:49:A:LEU:HB3  | 14       | 0.2           |
| (1,647)  | 1:45:A:LEU:HA   | 1:49:A:LEU:HA   | 19       | 0.2           |
| (1,406)  | 1:19:A:GLU:HB3  | 1:21:A:ILE:H    | 2        | 0.2           |
| (1,406)  | 1:19:A:GLU:HB3  | 1:21:A:ILE:H    | 19       | 0.2           |
| (1,360)  | 1:16:A:LEU:HB2  | 1:37:A:LEU:HG   | 12       | 0.2           |
| (1,1194) | 1:80:A:VAL:HA   | 1:83:A:GLN:HE21 | 4        | 0.19          |
| (1,1175) | 1:80:A:VAL:HA   | 1:84:A:GLN:HG2  | 7        | 0.19          |
| (1,1175) | 1:80:A:VAL:HA   | 1:84:A:GLN:HG2  | 15       | 0.19          |
| (1,1159) | 1:79:A:LEU:HA   | 1:83:A:GLN:HB3  | 10       | 0.19          |
| (1,1159) | 1:79:A:LEU:HA   | 1:83:A:GLN:HB3  | 16       | 0.19          |
| (1,1079) | 1:75:A:SER:HA   | 1:79:A:LEU:HB2  | 9        | 0.19          |
| (1,960)  | 1:69:A:HIS:HB2  | 1:79:A:LEU:HA   | 2        | 0.19          |
| (1,960)  | 1:69:A:HIS:HB2  | 1:79:A:LEU:HA   | 10       | 0.19          |
| (1,960)  | 1:69:A:HIS:HB2  | 1:79:A:LEU:HA   | 16       | 0.19          |
| (1,959)  | 1:69:A:HIS:HB2  | 1:79:A:LEU:H    | 7        | 0.19          |
| (1,959)  | 1:69:A:HIS:HB2  | 1:79:A:LEU:H    | 8        | 0.19          |
| (1,959)  | 1:69:A:HIS:HB2  | 1:79:A:LEU:H    | 10       | 0.19          |
| (1,951)  | 1:67:A:LYS:HA   | 1:71:A:LYS:H    | 9        | 0.19          |
| (1,857)  | 1:60:A:ASN:HB2  | 1:66:A:THR:HA   | 1        | 0.19          |
| (1,761)  | 1:52:A:LYS:HA   | 1:56:A:ASN:HB3  | 17       | 0.19          |
| (1,739)  | 1:51:A:LEU:HB3  | 1:54:A:ARG:HB3  | 1        | 0.19          |
| (1,736)  | 1:51:A:LEU:HB3  | 1:59:A:LEU:HG   | 3        | 0.19          |
| (1,736)  | 1:51:A:LEU:HB3  | 1:59:A:LEU:HG   | 7        | 0.19          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,736)  | 1:51:A:LEU:HB3  | 1:59:A:LEU:HG  | 20       | 0.19          |
| (1,688)  | 1:48:A:GLY:HA2  | 1:59:A:LEU:HB3 | 20       | 0.19          |
| (1,649)  | 1:45:A:LEU:HB2  | 1:49:A:LEU:HB3 | 5        | 0.19          |
| (1,649)  | 1:45:A:LEU:HB2  | 1:49:A:LEU:HB3 | 12       | 0.19          |
| (1,649)  | 1:45:A:LEU:HB2  | 1:49:A:LEU:HB3 | 20       | 0.19          |
| (1,535)  | 1:33:A:PHE:HA   | 1:39:A:LEU:HB3 | 14       | 0.19          |
| (1,406)  | 1:19:A:GLU:HB3  | 1:21:A:ILE:H   | 6        | 0.19          |
| (1,406)  | 1:19:A:GLU:HB3  | 1:21:A:ILE:H   | 10       | 0.19          |
| (1,364)  | 1:16:A:LEU:HD11 | 1:43:A:ASP:HA  | 14       | 0.19          |
| (1,364)  | 1:16:A:LEU:HD12 | 1:43:A:ASP:HA  | 14       | 0.19          |
| (1,364)  | 1:16:A:LEU:HD13 | 1:43:A:ASP:HA  | 14       | 0.19          |
| (1,364)  | 1:16:A:LEU:HD11 | 1:43:A:ASP:HA  | 15       | 0.19          |
| (1,364)  | 1:16:A:LEU:HD12 | 1:43:A:ASP:HA  | 15       | 0.19          |
| (1,364)  | 1:16:A:LEU:HD13 | 1:43:A:ASP:HA  | 15       | 0.19          |
| (1,360)  | 1:16:A:LEU:HB2  | 1:37:A:LEU:HG  | 1        | 0.19          |
| (1,360)  | 1:16:A:LEU:HB2  | 1:37:A:LEU:HG  | 6        | 0.19          |
| (1,1175) | 1:80:A:VAL:HA   | 1:84:A:GLN:HG2 | 3        | 0.18          |
| (1,1170) | 1:80:A:VAL:HB   | 1:82:A:ALA:H   | 11       | 0.18          |
| (1,1170) | 1:80:A:VAL:HB   | 1:82:A:ALA:H   | 18       | 0.18          |
| (1,1079) | 1:75:A:SER:HA   | 1:79:A:LEU:HB2 | 17       | 0.18          |
| (1,960)  | 1:69:A:HIS:HB2  | 1:79:A:LEU:HA  | 14       | 0.18          |
| (1,960)  | 1:69:A:HIS:HB2  | 1:79:A:LEU:HA  | 19       | 0.18          |
| (1,959)  | 1:69:A:HIS:HB2  | 1:79:A:LEU:H   | 11       | 0.18          |
| (1,959)  | 1:69:A:HIS:HB2  | 1:79:A:LEU:H   | 18       | 0.18          |
| (1,857)  | 1:60:A:ASN:HB2  | 1:66:A:THR:HA  | 3        | 0.18          |
| (1,796)  | 1:55:A:TYR:HB2  | 1:83:A:GLN:HB3 | 5        | 0.18          |
| (1,795)  | 1:55:A:TYR:HB3  | 1:57:A:ILE:HA  | 17       | 0.18          |
| (1,761)  | 1:52:A:LYS:HA   | 1:56:A:ASN:HB3 | 5        | 0.18          |
| (1,761)  | 1:52:A:LYS:HA   | 1:56:A:ASN:HB3 | 6        | 0.18          |
| (1,760)  | 1:52:A:LYS:HA   | 1:56:A:ASN:HB2 | 15       | 0.18          |
| (1,759)  | 1:52:A:LYS:HG2  | 1:58:A:HIS:H   | 10       | 0.18          |
| (1,737)  | 1:51:A:LEU:HA   | 1:57:A:ILE:H   | 1        | 0.18          |
| (1,737)  | 1:51:A:LEU:HA   | 1:57:A:ILE:H   | 3        | 0.18          |
| (1,737)  | 1:51:A:LEU:HA   | 1:57:A:ILE:H   | 20       | 0.18          |
| (1,736)  | 1:51:A:LEU:HB3  | 1:59:A:LEU:HG  | 4        | 0.18          |
| (1,651)  | 1:45:A:LEU:HA   | 1:48:A:GLY:HA2 | 9        | 0.18          |
| (1,651)  | 1:45:A:LEU:HA   | 1:48:A:GLY:HA2 | 17       | 0.18          |
| (1,649)  | 1:45:A:LEU:HB2  | 1:49:A:LEU:HB3 | 3        | 0.18          |
| (1,649)  | 1:45:A:LEU:HB2  | 1:49:A:LEU:HB3 | 7        | 0.18          |
| (1,647)  | 1:45:A:LEU:HA   | 1:49:A:LEU:HA  | 4        | 0.18          |
| (1,535)  | 1:33:A:PHE:HA   | 1:39:A:LEU:HB3 | 6        | 0.18          |
| (1,414)  | 1:21:A:ILE:HG13 | 1:25:A:ASP:HB2 | 6        | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,414)  | 1:21:A:ILE:HG13 | 1:25:A:ASP:HB2  | 17       | 0.18          |
| (1,414)  | 1:21:A:ILE:HG13 | 1:25:A:ASP:HB2  | 18       | 0.18          |
| (1,406)  | 1:19:A:GLU:HB3  | 1:21:A:ILE:H    | 15       | 0.18          |
| (1,364)  | 1:16:A:LEU:HD11 | 1:43:A:ASP:HA   | 16       | 0.18          |
| (1,364)  | 1:16:A:LEU:HD12 | 1:43:A:ASP:HA   | 16       | 0.18          |
| (1,364)  | 1:16:A:LEU:HD13 | 1:43:A:ASP:HA   | 16       | 0.18          |
| (1,360)  | 1:16:A:LEU:HB2  | 1:37:A:LEU:HG   | 11       | 0.18          |
| (1,337)  | 1:15:A:VAL:HB   | 1:51:A:LEU:HG   | 2        | 0.18          |
| (1,337)  | 1:15:A:VAL:HB   | 1:51:A:LEU:HG   | 10       | 0.18          |
| (1,337)  | 1:15:A:VAL:HB   | 1:51:A:LEU:HG   | 19       | 0.18          |
| (1,66)   | 1:5:A:ALA:HA    | 1:73:A:ILE:HG13 | 11       | 0.18          |
| (1,19)   | 1:4:A:LEU:HG    | 1:81:A:GLU:HA   | 4        | 0.18          |
| (1,13)   | 1:4:A:LEU:HG    | 1:8:A:LEU:HA    | 13       | 0.18          |
| (1,2)    | 1:2:A:SER:H     | 1:4:A:LEU:HB3   | 15       | 0.18          |
| (1,1170) | 1:80:A:VAL:HB   | 1:82:A:ALA:H    | 2        | 0.17          |
| (1,1170) | 1:80:A:VAL:HB   | 1:82:A:ALA:H    | 8        | 0.17          |
| (1,1170) | 1:80:A:VAL:HB   | 1:82:A:ALA:H    | 10       | 0.17          |
| (1,1169) | 1:80:A:VAL:HB   | 1:84:A:GLN:HG2  | 7        | 0.17          |
| (1,1169) | 1:80:A:VAL:HB   | 1:84:A:GLN:HG2  | 9        | 0.17          |
| (1,1159) | 1:79:A:LEU:HA   | 1:83:A:GLN:HB3  | 2        | 0.17          |
| (1,1159) | 1:79:A:LEU:HA   | 1:83:A:GLN:HB3  | 11       | 0.17          |
| (1,1091) | 1:76:A:LEU:HG   | 1:79:A:LEU:HB2  | 15       | 0.17          |
| (1,1079) | 1:75:A:SER:HA   | 1:79:A:LEU:HB2  | 11       | 0.17          |
| (1,1079) | 1:75:A:SER:HA   | 1:79:A:LEU:HB2  | 14       | 0.17          |
| (1,960)  | 1:69:A:HIS:HB2  | 1:79:A:LEU:HA   | 9        | 0.17          |
| (1,960)  | 1:69:A:HIS:HB2  | 1:79:A:LEU:HA   | 13       | 0.17          |
| (1,959)  | 1:69:A:HIS:HB2  | 1:79:A:LEU:H    | 2        | 0.17          |
| (1,886)  | 1:62:A:GLU:HA   | 1:67:A:LYS:HG2  | 17       | 0.17          |
| (1,877)  | 1:61:A:ALA:HA   | 1:66:A:THR:H    | 12       | 0.17          |
| (1,857)  | 1:60:A:ASN:HB2  | 1:66:A:THR:HA   | 20       | 0.17          |
| (1,800)  | 1:55:A:TYR:HB3  | 1:80:A:VAL:HA   | 4        | 0.17          |
| (1,761)  | 1:52:A:LYS:HA   | 1:56:A:ASN:HB3  | 10       | 0.17          |
| (1,760)  | 1:52:A:LYS:HA   | 1:56:A:ASN:HB2  | 1        | 0.17          |
| (1,760)  | 1:52:A:LYS:HA   | 1:56:A:ASN:HB2  | 9        | 0.17          |
| (1,760)  | 1:52:A:LYS:HA   | 1:56:A:ASN:HB2  | 13       | 0.17          |
| (1,759)  | 1:52:A:LYS:HG2  | 1:58:A:HIS:H    | 11       | 0.17          |
| (1,739)  | 1:51:A:LEU:HB3  | 1:54:A:ARG:HB3  | 13       | 0.17          |
| (1,738)  | 1:51:A:LEU:HA   | 1:57:A:ILE:HB   | 10       | 0.17          |
| (1,737)  | 1:51:A:LEU:HA   | 1:57:A:ILE:H    | 4        | 0.17          |
| (1,737)  | 1:51:A:LEU:HA   | 1:57:A:ILE:H    | 7        | 0.17          |
| (1,736)  | 1:51:A:LEU:HB3  | 1:59:A:LEU:HG   | 19       | 0.17          |
| (1,722)  | 1:50:A:ALA:HA   | 1:52:A:LYS:HB3  | 13       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,689)  | 1:48:A:GLY:HA3  | 1:52:A:LYS:HB2  | 3        | 0.17          |
| (1,689)  | 1:48:A:GLY:HA3  | 1:52:A:LYS:HB2  | 9        | 0.17          |
| (1,649)  | 1:45:A:LEU:HB2  | 1:49:A:LEU:HB3  | 6        | 0.17          |
| (1,649)  | 1:45:A:LEU:HB2  | 1:49:A:LEU:HB3  | 18       | 0.17          |
| (1,618)  | 1:43:A:ASP:HB3  | 1:46:A:GLU:H    | 6        | 0.17          |
| (1,406)  | 1:19:A:GLU:HB3  | 1:21:A:ILE:H    | 17       | 0.17          |
| (1,387)  | 1:18:A:LEU:HB2  | 1:21:A:ILE:HG12 | 14       | 0.17          |
| (1,364)  | 1:16:A:LEU:HD11 | 1:43:A:ASP:HA   | 11       | 0.17          |
| (1,364)  | 1:16:A:LEU:HD12 | 1:43:A:ASP:HA   | 11       | 0.17          |
| (1,364)  | 1:16:A:LEU:HD13 | 1:43:A:ASP:HA   | 11       | 0.17          |
| (1,337)  | 1:15:A:VAL:HB   | 1:51:A:LEU:HG   | 11       | 0.17          |
| (1,337)  | 1:15:A:VAL:HB   | 1:51:A:LEU:HG   | 14       | 0.17          |
| (1,308)  | 1:13:A:ILE:HA   | 1:18:A:LEU:HA   | 14       | 0.17          |
| (1,26)   | 1:4:A:LEU:HB3   | 1:81:A:GLU:HA   | 15       | 0.17          |
| (1,16)   | 1:4:A:LEU:HB2   | 1:77:A:VAL:HB   | 15       | 0.17          |
| (1,13)   | 1:4:A:LEU:HG    | 1:8:A:LEU:HA    | 6        | 0.17          |
| (1,13)   | 1:4:A:LEU:HG    | 1:8:A:LEU:HA    | 15       | 0.17          |
| (1,2)    | 1:2:A:SER:H     | 1:4:A:LEU:HB3   | 1        | 0.17          |
| (1,1198) | 1:81:A:GLU:HA   | 1:83:A:GLN:HG2  | 5        | 0.16          |
| (1,1170) | 1:80:A:VAL:HB   | 1:82:A:ALA:H    | 12       | 0.16          |
| (1,1169) | 1:80:A:VAL:HB   | 1:84:A:GLN:HG2  | 1        | 0.16          |
| (1,1169) | 1:80:A:VAL:HB   | 1:84:A:GLN:HG2  | 6        | 0.16          |
| (1,1159) | 1:79:A:LEU:HA   | 1:83:A:GLN:HB3  | 5        | 0.16          |
| (1,1159) | 1:79:A:LEU:HA   | 1:83:A:GLN:HB3  | 18       | 0.16          |
| (1,1094) | 1:76:A:LEU:HB3  | 1:79:A:LEU:H    | 3        | 0.16          |
| (1,1094) | 1:76:A:LEU:HB3  | 1:79:A:LEU:H    | 12       | 0.16          |
| (1,1091) | 1:76:A:LEU:HG   | 1:79:A:LEU:HB2  | 3        | 0.16          |
| (1,1079) | 1:75:A:SER:HA   | 1:79:A:LEU:HB2  | 13       | 0.16          |
| (1,1079) | 1:75:A:SER:HA   | 1:79:A:LEU:HB2  | 16       | 0.16          |
| (1,1079) | 1:75:A:SER:HA   | 1:79:A:LEU:HB2  | 19       | 0.16          |
| (1,1035) | 1:73:A:ILE:HG12 | 1:76:A:LEU:HB2  | 1        | 0.16          |
| (1,986)  | 1:70:A:PHE:HB3  | 1:75:A:SER:HB2  | 9        | 0.16          |
| (1,986)  | 1:70:A:PHE:HB3  | 1:75:A:SER:HB2  | 17       | 0.16          |
| (1,960)  | 1:69:A:HIS:HB2  | 1:79:A:LEU:HA   | 6        | 0.16          |
| (1,959)  | 1:69:A:HIS:HB2  | 1:79:A:LEU:H    | 13       | 0.16          |
| (1,959)  | 1:69:A:HIS:HB2  | 1:79:A:LEU:H    | 16       | 0.16          |
| (1,892)  | 1:63:A:SER:HA   | 1:67:A:LYS:HG2  | 9        | 0.16          |
| (1,891)  | 1:63:A:SER:H    | 1:65:A:GLU:H    | 7        | 0.16          |
| (1,858)  | 1:60:A:ASN:HA   | 1:66:A:THR:H    | 5        | 0.16          |
| (1,857)  | 1:60:A:ASN:HB2  | 1:66:A:THR:HA   | 12       | 0.16          |
| (1,847)  | 1:58:A:HIS:H    | 1:83:A:GLN:HE22 | 4        | 0.16          |
| (1,832)  | 1:57:A:ILE:HB   | 1:59:A:LEU:HG   | 6        | 0.16          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,832)  | 1:57:A:ILE:HB  | 1:59:A:LEU:HG   | 10       | 0.16          |
| (1,832)  | 1:57:A:ILE:HB  | 1:59:A:LEU:HG   | 13       | 0.16          |
| (1,794)  | 1:55:A:TYR:HB2 | 1:84:A:GLN:HG2  | 1        | 0.16          |
| (1,794)  | 1:55:A:TYR:HB2 | 1:84:A:GLN:HG2  | 14       | 0.16          |
| (1,794)  | 1:55:A:TYR:HB2 | 1:84:A:GLN:HG2  | 17       | 0.16          |
| (1,784)  | 1:53:A:LYS:HA  | 1:55:A:TYR:H    | 10       | 0.16          |
| (1,772)  | 1:52:A:LYS:H   | 1:53:A:LYS:HG2  | 19       | 0.16          |
| (1,760)  | 1:52:A:LYS:HA  | 1:56:A:ASN:HB2  | 14       | 0.16          |
| (1,759)  | 1:52:A:LYS:HG2 | 1:58:A:HIS:H    | 2        | 0.16          |
| (1,759)  | 1:52:A:LYS:HG2 | 1:58:A:HIS:H    | 8        | 0.16          |
| (1,759)  | 1:52:A:LYS:HG2 | 1:58:A:HIS:H    | 12       | 0.16          |
| (1,759)  | 1:52:A:LYS:HG2 | 1:58:A:HIS:H    | 15       | 0.16          |
| (1,739)  | 1:51:A:LEU:HB3 | 1:54:A:ARG:HB3  | 11       | 0.16          |
| (1,736)  | 1:51:A:LEU:HB3 | 1:59:A:LEU:HG   | 15       | 0.16          |
| (1,724)  | 1:50:A:ALA:H   | 1:52:A:LYS:HB3  | 15       | 0.16          |
| (1,710)  | 1:49:A:LEU:HA  | 1:52:A:LYS:HG2  | 15       | 0.16          |
| (1,709)  | 1:49:A:LEU:HA  | 1:59:A:LEU:HG   | 10       | 0.16          |
| (1,709)  | 1:49:A:LEU:HA  | 1:59:A:LEU:HG   | 11       | 0.16          |
| (1,688)  | 1:48:A:GLY:HA2 | 1:59:A:LEU:HB3  | 15       | 0.16          |
| (1,618)  | 1:43:A:ASP:HB3 | 1:46:A:GLU:H    | 14       | 0.16          |
| (1,600)  | 1:41:A:SER:HA  | 1:45:A:LEU:H    | 1        | 0.16          |
| (1,600)  | 1:41:A:SER:HA  | 1:45:A:LEU:H    | 8        | 0.16          |
| (1,572)  | 1:39:A:LEU:HA  | 1:43:A:ASP:H    | 16       | 0.16          |
| (1,535)  | 1:33:A:PHE:HA  | 1:39:A:LEU:HB3  | 17       | 0.16          |
| (1,505)  | 1:31:A:PRO:HB3 | 1:34:A:GLY:HA2  | 11       | 0.16          |
| (1,479)  | 1:29:A:GLU:HA  | 1:72:A:SER:H    | 15       | 0.16          |
| (1,387)  | 1:18:A:LEU:HB2 | 1:21:A:ILE:HG12 | 8        | 0.16          |
| (1,387)  | 1:18:A:LEU:HB2 | 1:21:A:ILE:HG12 | 11       | 0.16          |
| (1,337)  | 1:15:A:VAL:HB  | 1:51:A:LEU:HG   | 7        | 0.16          |
| (1,258)  | 1:11:A:MET:HB2 | 1:15:A:VAL:HB   | 5        | 0.16          |
| (1,182)  | 1:9:A:LYS:HA   | 1:13:A:ILE:HB   | 4        | 0.16          |
| (1,68)   | 1:5:A:ALA:HA   | 1:9:A:LYS:HB2   | 10       | 0.16          |
| (1,68)   | 1:5:A:ALA:HA   | 1:9:A:LYS:HB2   | 15       | 0.16          |
| (1,68)   | 1:5:A:ALA:HA   | 1:9:A:LYS:HB2   | 16       | 0.16          |
| (1,66)   | 1:5:A:ALA:HA   | 1:73:A:ILE:HG13 | 18       | 0.16          |
| (1,19)   | 1:4:A:LEU:HG   | 1:81:A:GLU:HA   | 9        | 0.16          |
| (1,19)   | 1:4:A:LEU:HG   | 1:81:A:GLU:HA   | 20       | 0.16          |
| (1,15)   | 1:4:A:LEU:HG   | 1:7:A:GLU:HB2   | 2        | 0.16          |
| (1,13)   | 1:4:A:LEU:HG   | 1:8:A:LEU:HA    | 16       | 0.16          |
| (1,2)    | 1:2:A:SER:H    | 1:4:A:LEU:HB3   | 13       | 0.16          |
| (1,1198) | 1:81:A:GLU:HA  | 1:83:A:GLN:HG2  | 16       | 0.15          |
| (1,1175) | 1:80:A:VAL:HA  | 1:84:A:GLN:HG2  | 5        | 0.15          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1175) | 1:80:A:VAL:HA   | 1:84:A:GLN:HG2 | 14       | 0.15          |
| (1,1170) | 1:80:A:VAL:HB   | 1:82:A:ALA:H   | 6        | 0.15          |
| (1,1170) | 1:80:A:VAL:HB   | 1:82:A:ALA:H   | 13       | 0.15          |
| (1,1170) | 1:80:A:VAL:HB   | 1:82:A:ALA:H   | 16       | 0.15          |
| (1,1169) | 1:80:A:VAL:HB   | 1:84:A:GLN:HG2 | 4        | 0.15          |
| (1,1169) | 1:80:A:VAL:HB   | 1:84:A:GLN:HG2 | 13       | 0.15          |
| (1,1169) | 1:80:A:VAL:HB   | 1:84:A:GLN:HG2 | 14       | 0.15          |
| (1,1169) | 1:80:A:VAL:HB   | 1:84:A:GLN:HG2 | 17       | 0.15          |
| (1,1169) | 1:80:A:VAL:HB   | 1:84:A:GLN:HG2 | 19       | 0.15          |
| (1,1169) | 1:80:A:VAL:HB   | 1:84:A:GLN:HG2 | 20       | 0.15          |
| (1,1159) | 1:79:A:LEU:HA   | 1:83:A:GLN:HB3 | 12       | 0.15          |
| (1,1158) | 1:79:A:LEU:HB3  | 1:82:A:ALA:H   | 12       | 0.15          |
| (1,1094) | 1:76:A:LEU:HB3  | 1:79:A:LEU:H   | 5        | 0.15          |
| (1,1094) | 1:76:A:LEU:HB3  | 1:79:A:LEU:H   | 20       | 0.15          |
| (1,1091) | 1:76:A:LEU:HG   | 1:79:A:LEU:HB2 | 5        | 0.15          |
| (1,1091) | 1:76:A:LEU:HG   | 1:79:A:LEU:HB2 | 7        | 0.15          |
| (1,1091) | 1:76:A:LEU:HG   | 1:79:A:LEU:HB2 | 20       | 0.15          |
| (1,1079) | 1:75:A:SER:HA   | 1:79:A:LEU:HB2 | 2        | 0.15          |
| (1,1079) | 1:75:A:SER:HA   | 1:79:A:LEU:HB2 | 6        | 0.15          |
| (1,1079) | 1:75:A:SER:HA   | 1:79:A:LEU:HB2 | 8        | 0.15          |
| (1,1035) | 1:73:A:ILE:HG12 | 1:76:A:LEU:HB2 | 3        | 0.15          |
| (1,986)  | 1:70:A:PHE:HB3  | 1:75:A:SER:HB2 | 6        | 0.15          |
| (1,962)  | 1:69:A:HIS:HB2  | 1:76:A:LEU:HG  | 1        | 0.15          |
| (1,962)  | 1:69:A:HIS:HB2  | 1:76:A:LEU:HG  | 10       | 0.15          |
| (1,960)  | 1:69:A:HIS:HB2  | 1:79:A:LEU:HA  | 4        | 0.15          |
| (1,960)  | 1:69:A:HIS:HB2  | 1:79:A:LEU:HA  | 17       | 0.15          |
| (1,959)  | 1:69:A:HIS:HB2  | 1:79:A:LEU:H   | 6        | 0.15          |
| (1,959)  | 1:69:A:HIS:HB2  | 1:79:A:LEU:H   | 19       | 0.15          |
| (1,940)  | 1:66:A:THR:H    | 1:70:A:PHE:H   | 9        | 0.15          |
| (1,940)  | 1:66:A:THR:H    | 1:70:A:PHE:H   | 17       | 0.15          |
| (1,892)  | 1:63:A:SER:HA   | 1:67:A:LYS:HG2 | 6        | 0.15          |
| (1,892)  | 1:63:A:SER:HA   | 1:67:A:LYS:HG2 | 11       | 0.15          |
| (1,890)  | 1:63:A:SER:H    | 1:65:A:GLU:HB2 | 13       | 0.15          |
| (1,890)  | 1:63:A:SER:H    | 1:65:A:GLU:HB3 | 13       | 0.15          |
| (1,877)  | 1:61:A:ALA:HA   | 1:66:A:THR:H   | 5        | 0.15          |
| (1,833)  | 1:57:A:ILE:HA   | 1:59:A:LEU:H   | 9        | 0.15          |
| (1,832)  | 1:57:A:ILE:HB   | 1:59:A:LEU:HG  | 16       | 0.15          |
| (1,829)  | 1:57:A:ILE:HA   | 1:80:A:VAL:HA  | 15       | 0.15          |
| (1,829)  | 1:57:A:ILE:HA   | 1:80:A:VAL:HA  | 17       | 0.15          |
| (1,796)  | 1:55:A:TYR:HB2  | 1:83:A:GLN:HB3 | 17       | 0.15          |
| (1,794)  | 1:55:A:TYR:HB2  | 1:84:A:GLN:HG2 | 3        | 0.15          |
| (1,761)  | 1:52:A:LYS:HA   | 1:56:A:ASN:HB3 | 4        | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,760) | 1:52:A:LYS:HA   | 1:56:A:ASN:HB2  | 7        | 0.15          |
| (1,760) | 1:52:A:LYS:HA   | 1:56:A:ASN:HB2  | 19       | 0.15          |
| (1,760) | 1:52:A:LYS:HA   | 1:56:A:ASN:HB2  | 20       | 0.15          |
| (1,759) | 1:52:A:LYS:HG2  | 1:58:A:HIS:H    | 13       | 0.15          |
| (1,739) | 1:51:A:LEU:HB3  | 1:54:A:ARG:HB3  | 2        | 0.15          |
| (1,738) | 1:51:A:LEU:HA   | 1:57:A:ILE:HB   | 18       | 0.15          |
| (1,737) | 1:51:A:LEU:HA   | 1:57:A:ILE:H    | 18       | 0.15          |
| (1,737) | 1:51:A:LEU:HA   | 1:57:A:ILE:H    | 19       | 0.15          |
| (1,736) | 1:51:A:LEU:HB3  | 1:59:A:LEU:HG   | 12       | 0.15          |
| (1,707) | 1:49:A:LEU:HA   | 1:53:A:LYS:H    | 2        | 0.15          |
| (1,707) | 1:49:A:LEU:HA   | 1:53:A:LYS:H    | 12       | 0.15          |
| (1,689) | 1:48:A:GLY:HA3  | 1:52:A:LYS:HB2  | 1        | 0.15          |
| (1,688) | 1:48:A:GLY:HA2  | 1:59:A:LEU:HB3  | 7        | 0.15          |
| (1,687) | 1:48:A:GLY:HA2  | 1:59:A:LEU:HB2  | 15       | 0.15          |
| (1,675) | 1:47:A:LEU:HA   | 1:51:A:LEU:HA   | 10       | 0.15          |
| (1,674) | 1:47:A:LEU:HG   | 1:51:A:LEU:HB3  | 18       | 0.15          |
| (1,652) | 1:45:A:LEU:HA   | 1:49:A:LEU:HB3  | 10       | 0.15          |
| (1,651) | 1:45:A:LEU:HA   | 1:48:A:GLY:HA2  | 2        | 0.15          |
| (1,651) | 1:45:A:LEU:HA   | 1:48:A:GLY:HA2  | 11       | 0.15          |
| (1,648) | 1:45:A:LEU:HB2  | 1:49:A:LEU:H    | 1        | 0.15          |
| (1,647) | 1:45:A:LEU:HA   | 1:49:A:LEU:HA   | 2        | 0.15          |
| (1,647) | 1:45:A:LEU:HA   | 1:49:A:LEU:HA   | 3        | 0.15          |
| (1,647) | 1:45:A:LEU:HA   | 1:49:A:LEU:HA   | 8        | 0.15          |
| (1,647) | 1:45:A:LEU:HA   | 1:49:A:LEU:HA   | 10       | 0.15          |
| (1,647) | 1:45:A:LEU:HA   | 1:49:A:LEU:HA   | 13       | 0.15          |
| (1,628) | 1:44:A:ALA:HA   | 1:48:A:GLY:HA3  | 3        | 0.15          |
| (1,628) | 1:44:A:ALA:HA   | 1:48:A:GLY:HA3  | 5        | 0.15          |
| (1,618) | 1:43:A:ASP:HB3  | 1:46:A:GLU:H    | 15       | 0.15          |
| (1,600) | 1:41:A:SER:HA   | 1:45:A:LEU:H    | 13       | 0.15          |
| (1,572) | 1:39:A:LEU:HA   | 1:43:A:ASP:H    | 6        | 0.15          |
| (1,517) | 1:32:A:LEU:HB2  | 1:39:A:LEU:H    | 12       | 0.15          |
| (1,499) | 1:29:A:GLU:HG3  | 1:74:A:GLN:HA   | 3        | 0.15          |
| (1,480) | 1:29:A:GLU:H    | 1:74:A:GLN:HB3  | 4        | 0.15          |
| (1,414) | 1:21:A:ILE:HG13 | 1:25:A:ASP:HB2  | 9        | 0.15          |
| (1,387) | 1:18:A:LEU:HB2  | 1:21:A:ILE:HG12 | 7        | 0.15          |
| (1,364) | 1:16:A:LEU:HD11 | 1:43:A:ASP:HA   | 6        | 0.15          |
| (1,364) | 1:16:A:LEU:HD12 | 1:43:A:ASP:HA   | 6        | 0.15          |
| (1,364) | 1:16:A:LEU:HD13 | 1:43:A:ASP:HA   | 6        | 0.15          |
| (1,360) | 1:16:A:LEU:HB2  | 1:37:A:LEU:HG   | 7        | 0.15          |
| (1,337) | 1:15:A:VAL:HB   | 1:51:A:LEU:HG   | 8        | 0.15          |
| (1,337) | 1:15:A:VAL:HB   | 1:51:A:LEU:HG   | 12       | 0.15          |
| (1,258) | 1:11:A:MET:HB2  | 1:15:A:VAL:HB   | 11       | 0.15          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,258)  | 1:11:A:MET:HB2 | 1:15:A:VAL:HB   | 16       | 0.15          |
| (1,125)  | 1:8:A:LEU:HB3  | 1:77:A:VAL:HA   | 7        | 0.15          |
| (1,68)   | 1:5:A:ALA:HA   | 1:9:A:LYS:HB2   | 3        | 0.15          |
| (1,66)   | 1:5:A:ALA:HA   | 1:73:A:ILE:HG13 | 5        | 0.15          |
| (1,66)   | 1:5:A:ALA:HA   | 1:73:A:ILE:HG13 | 8        | 0.15          |
| (1,66)   | 1:5:A:ALA:HA   | 1:73:A:ILE:HG13 | 12       | 0.15          |
| (1,66)   | 1:5:A:ALA:HA   | 1:73:A:ILE:HG13 | 13       | 0.15          |
| (1,19)   | 1:4:A:LEU:HG   | 1:81:A:GLU:HA   | 15       | 0.15          |
| (1,19)   | 1:4:A:LEU:HG   | 1:81:A:GLU:HA   | 17       | 0.15          |
| (1,18)   | 1:4:A:LEU:HA   | 1:8:A:LEU:HA    | 20       | 0.15          |
| (1,15)   | 1:4:A:LEU:HG   | 1:7:A:GLU:HB2   | 6        | 0.15          |
| (1,13)   | 1:4:A:LEU:HG   | 1:8:A:LEU:HA    | 2        | 0.15          |
| (1,13)   | 1:4:A:LEU:HG   | 1:8:A:LEU:HA    | 9        | 0.15          |
| (1,13)   | 1:4:A:LEU:HG   | 1:8:A:LEU:HA    | 11       | 0.15          |
| (1,7)    | 1:3:A:ASN:H    | 1:84:A:GLN:HE22 | 10       | 0.15          |
| (1,7)    | 1:3:A:ASN:H    | 1:84:A:GLN:HE22 | 12       | 0.15          |
| (1,2)    | 1:2:A:SER:H    | 1:4:A:LEU:HB3   | 2        | 0.15          |
| (1,2)    | 1:2:A:SER:H    | 1:4:A:LEU:HB3   | 3        | 0.15          |
| (1,2)    | 1:2:A:SER:H    | 1:4:A:LEU:HB3   | 7        | 0.15          |
| (2,69)   | 1:77:A:VAL:O   | 1:81:A:GLU:N    | 9        | 0.14          |
| (2,69)   | 1:77:A:VAL:O   | 1:81:A:GLU:N    | 11       | 0.14          |
| (2,69)   | 1:77:A:VAL:O   | 1:81:A:GLU:N    | 14       | 0.14          |
| (2,69)   | 1:77:A:VAL:O   | 1:81:A:GLU:N    | 16       | 0.14          |
| (2,61)   | 1:73:A:ILE:O   | 1:77:A:VAL:N    | 2        | 0.14          |
| (2,61)   | 1:73:A:ILE:O   | 1:77:A:VAL:N    | 5        | 0.14          |
| (2,61)   | 1:73:A:ILE:O   | 1:77:A:VAL:N    | 7        | 0.14          |
| (2,61)   | 1:73:A:ILE:O   | 1:77:A:VAL:N    | 8        | 0.14          |
| (2,61)   | 1:73:A:ILE:O   | 1:77:A:VAL:N    | 9        | 0.14          |
| (2,61)   | 1:73:A:ILE:O   | 1:77:A:VAL:N    | 12       | 0.14          |
| (2,61)   | 1:73:A:ILE:O   | 1:77:A:VAL:N    | 13       | 0.14          |
| (2,61)   | 1:73:A:ILE:O   | 1:77:A:VAL:N    | 14       | 0.14          |
| (2,61)   | 1:73:A:ILE:O   | 1:77:A:VAL:N    | 17       | 0.14          |
| (2,61)   | 1:73:A:ILE:O   | 1:77:A:VAL:N    | 18       | 0.14          |
| (2,61)   | 1:73:A:ILE:O   | 1:77:A:VAL:N    | 19       | 0.14          |
| (2,49)   | 1:52:A:LYS:O   | 1:56:A:ASN:N    | 3        | 0.14          |
| (1,1217) | 1:83:A:GLN:H   | 1:85:A:LYS:H    | 10       | 0.14          |
| (1,1217) | 1:83:A:GLN:H   | 1:85:A:LYS:H    | 11       | 0.14          |
| (1,1175) | 1:80:A:VAL:HA  | 1:84:A:GLN:HG2  | 13       | 0.14          |
| (1,1175) | 1:80:A:VAL:HA  | 1:84:A:GLN:HG2  | 17       | 0.14          |
| (1,1169) | 1:80:A:VAL:HB  | 1:84:A:GLN:HG2  | 3        | 0.14          |
| (1,1169) | 1:80:A:VAL:HB  | 1:84:A:GLN:HG2  | 16       | 0.14          |
| (1,1168) | 1:80:A:VAL:HA  | 1:83:A:GLN:HA   | 4        | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1159) | 1:79:A:LEU:HA   | 1:83:A:GLN:HB3  | 8        | 0.14          |
| (1,1158) | 1:79:A:LEU:HB3  | 1:82:A:ALA:H    | 11       | 0.14          |
| (1,1157) | 1:79:A:LEU:H    | 1:81:A:GLU:H    | 13       | 0.14          |
| (1,1094) | 1:76:A:LEU:HB3  | 1:79:A:LEU:H    | 7        | 0.14          |
| (1,1094) | 1:76:A:LEU:HB3  | 1:79:A:LEU:H    | 15       | 0.14          |
| (1,1091) | 1:76:A:LEU:HG   | 1:79:A:LEU:HB2  | 12       | 0.14          |
| (1,1080) | 1:75:A:SER:HB3  | 1:79:A:LEU:HG   | 12       | 0.14          |
| (1,1079) | 1:75:A:SER:HA   | 1:79:A:LEU:HB2  | 1        | 0.14          |
| (1,1079) | 1:75:A:SER:HA   | 1:79:A:LEU:HB2  | 4        | 0.14          |
| (1,1079) | 1:75:A:SER:HA   | 1:79:A:LEU:HB2  | 10       | 0.14          |
| (1,1078) | 1:75:A:SER:HB2  | 1:79:A:LEU:H    | 7        | 0.14          |
| (1,1035) | 1:73:A:ILE:HG12 | 1:76:A:LEU:HB2  | 10       | 0.14          |
| (1,986)  | 1:70:A:PHE:HB3  | 1:75:A:SER:HB2  | 16       | 0.14          |
| (1,985)  | 1:70:A:PHE:HB2  | 1:75:A:SER:HB2  | 6        | 0.14          |
| (1,985)  | 1:70:A:PHE:HB2  | 1:75:A:SER:HB2  | 9        | 0.14          |
| (1,985)  | 1:70:A:PHE:HB2  | 1:75:A:SER:HB2  | 17       | 0.14          |
| (1,962)  | 1:69:A:HIS:HB2  | 1:76:A:LEU:HG   | 16       | 0.14          |
| (1,962)  | 1:69:A:HIS:HB2  | 1:76:A:LEU:HG   | 18       | 0.14          |
| (1,961)  | 1:69:A:HIS:H    | 1:75:A:SER:HB2  | 3        | 0.14          |
| (1,961)  | 1:69:A:HIS:H    | 1:75:A:SER:HB2  | 12       | 0.14          |
| (1,961)  | 1:69:A:HIS:H    | 1:75:A:SER:HB2  | 20       | 0.14          |
| (1,960)  | 1:69:A:HIS:HB2  | 1:79:A:LEU:HA   | 1        | 0.14          |
| (1,959)  | 1:69:A:HIS:HB2  | 1:79:A:LEU:H    | 14       | 0.14          |
| (1,891)  | 1:63:A:SER:H    | 1:65:A:GLU:H    | 3        | 0.14          |
| (1,891)  | 1:63:A:SER:H    | 1:65:A:GLU:H    | 10       | 0.14          |
| (1,891)  | 1:63:A:SER:H    | 1:65:A:GLU:H    | 19       | 0.14          |
| (1,891)  | 1:63:A:SER:H    | 1:65:A:GLU:H    | 20       | 0.14          |
| (1,886)  | 1:62:A:GLU:HA   | 1:67:A:LYS:HG2  | 2        | 0.14          |
| (1,886)  | 1:62:A:GLU:HA   | 1:67:A:LYS:HG2  | 8        | 0.14          |
| (1,886)  | 1:62:A:GLU:HA   | 1:67:A:LYS:HG2  | 10       | 0.14          |
| (1,886)  | 1:62:A:GLU:HA   | 1:67:A:LYS:HG2  | 12       | 0.14          |
| (1,877)  | 1:61:A:ALA:HA   | 1:66:A:THR:H    | 6        | 0.14          |
| (1,858)  | 1:60:A:ASN:HA   | 1:66:A:THR:H    | 3        | 0.14          |
| (1,858)  | 1:60:A:ASN:HA   | 1:66:A:THR:H    | 12       | 0.14          |
| (1,857)  | 1:60:A:ASN:HB2  | 1:66:A:THR:HA   | 6        | 0.14          |
| (1,857)  | 1:60:A:ASN:HB2  | 1:66:A:THR:HA   | 14       | 0.14          |
| (1,850)  | 1:59:A:LEU:HB2  | 1:61:A:ALA:HA   | 9        | 0.14          |
| (1,832)  | 1:57:A:ILE:HB   | 1:59:A:LEU:HG   | 5        | 0.14          |
| (1,832)  | 1:57:A:ILE:HB   | 1:59:A:LEU:HG   | 8        | 0.14          |
| (1,832)  | 1:57:A:ILE:HB   | 1:59:A:LEU:HG   | 18       | 0.14          |
| (1,797)  | 1:55:A:TYR:HB2  | 1:57:A:ILE:HG12 | 6        | 0.14          |
| (1,797)  | 1:55:A:TYR:HB2  | 1:57:A:ILE:HG13 | 6        | 0.14          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,796) | 1:55:A:TYR:HB2 | 1:83:A:GLN:HB3 | 14       | 0.14          |
| (1,796) | 1:55:A:TYR:HB2 | 1:83:A:GLN:HB3 | 16       | 0.14          |
| (1,795) | 1:55:A:TYR:HB3 | 1:57:A:ILE:HA  | 5        | 0.14          |
| (1,795) | 1:55:A:TYR:HB3 | 1:57:A:ILE:HA  | 14       | 0.14          |
| (1,789) | 1:54:A:ARG:H   | 1:55:A:TYR:HA  | 18       | 0.14          |
| (1,784) | 1:53:A:LYS:HA  | 1:55:A:TYR:H   | 2        | 0.14          |
| (1,760) | 1:52:A:LYS:HA  | 1:56:A:ASN:HB2 | 3        | 0.14          |
| (1,759) | 1:52:A:LYS:HG2 | 1:58:A:HIS:H   | 5        | 0.14          |
| (1,759) | 1:52:A:LYS:HG2 | 1:58:A:HIS:H   | 6        | 0.14          |
| (1,758) | 1:52:A:LYS:HG3 | 1:57:A:ILE:H   | 14       | 0.14          |
| (1,739) | 1:51:A:LEU:HB3 | 1:54:A:ARG:HB3 | 3        | 0.14          |
| (1,739) | 1:51:A:LEU:HB3 | 1:54:A:ARG:HB3 | 12       | 0.14          |
| (1,736) | 1:51:A:LEU:HB3 | 1:59:A:LEU:HG  | 2        | 0.14          |
| (1,736) | 1:51:A:LEU:HB3 | 1:59:A:LEU:HG  | 11       | 0.14          |
| (1,736) | 1:51:A:LEU:HB3 | 1:59:A:LEU:HG  | 14       | 0.14          |
| (1,722) | 1:50:A:ALA:HA  | 1:52:A:LYS:HB3 | 15       | 0.14          |
| (1,711) | 1:49:A:LEU:HA  | 1:53:A:LYS:HG2 | 19       | 0.14          |
| (1,710) | 1:49:A:LEU:HA  | 1:52:A:LYS:HG2 | 14       | 0.14          |
| (1,710) | 1:49:A:LEU:HA  | 1:52:A:LYS:HG2 | 20       | 0.14          |
| (1,707) | 1:49:A:LEU:HA  | 1:53:A:LYS:H   | 3        | 0.14          |
| (1,707) | 1:49:A:LEU:HA  | 1:53:A:LYS:H   | 8        | 0.14          |
| (1,693) | 1:48:A:GLY:HA3 | 1:51:A:LEU:HG  | 7        | 0.14          |
| (1,693) | 1:48:A:GLY:HA3 | 1:51:A:LEU:HG  | 15       | 0.14          |
| (1,692) | 1:48:A:GLY:HA2 | 1:51:A:LEU:HA  | 15       | 0.14          |
| (1,689) | 1:48:A:GLY:HA3 | 1:52:A:LYS:HB2 | 4        | 0.14          |
| (1,689) | 1:48:A:GLY:HA3 | 1:52:A:LYS:HB2 | 5        | 0.14          |
| (1,689) | 1:48:A:GLY:HA3 | 1:52:A:LYS:HB2 | 17       | 0.14          |
| (1,689) | 1:48:A:GLY:HA3 | 1:52:A:LYS:HB2 | 20       | 0.14          |
| (1,688) | 1:48:A:GLY:HA2 | 1:59:A:LEU:HB3 | 16       | 0.14          |
| (1,687) | 1:48:A:GLY:HA2 | 1:59:A:LEU:HB2 | 1        | 0.14          |
| (1,687) | 1:48:A:GLY:HA2 | 1:59:A:LEU:HB2 | 10       | 0.14          |
| (1,687) | 1:48:A:GLY:HA2 | 1:59:A:LEU:HB2 | 16       | 0.14          |
| (1,674) | 1:47:A:LEU:HG  | 1:51:A:LEU:HB3 | 13       | 0.14          |
| (1,673) | 1:47:A:LEU:HB3 | 1:51:A:LEU:HG  | 9        | 0.14          |
| (1,673) | 1:47:A:LEU:HB3 | 1:51:A:LEU:HG  | 17       | 0.14          |
| (1,648) | 1:45:A:LEU:HB2 | 1:49:A:LEU:H   | 5        | 0.14          |
| (1,647) | 1:45:A:LEU:HA  | 1:49:A:LEU:HA  | 1        | 0.14          |
| (1,647) | 1:45:A:LEU:HA  | 1:49:A:LEU:HA  | 9        | 0.14          |
| (1,647) | 1:45:A:LEU:HA  | 1:49:A:LEU:HA  | 15       | 0.14          |
| (1,647) | 1:45:A:LEU:HA  | 1:49:A:LEU:HA  | 17       | 0.14          |
| (1,631) | 1:44:A:ALA:HA  | 1:47:A:LEU:HG  | 7        | 0.14          |
| (1,618) | 1:43:A:ASP:HB3 | 1:46:A:GLU:H   | 16       | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,600) | 1:41:A:SER:HA   | 1:45:A:LEU:H    | 3        | 0.14          |
| (1,600) | 1:41:A:SER:HA   | 1:45:A:LEU:H    | 19       | 0.14          |
| (1,571) | 1:39:A:LEU:HB2  | 1:43:A:ASP:H    | 4        | 0.14          |
| (1,559) | 1:37:A:LEU:HB2  | 1:39:A:LEU:HA   | 12       | 0.14          |
| (1,535) | 1:33:A:PHE:HA   | 1:39:A:LEU:HB3  | 9        | 0.14          |
| (1,517) | 1:32:A:LEU:HB2  | 1:39:A:LEU:H    | 7        | 0.14          |
| (1,503) | 1:31:A:PRO:HB2  | 1:35:A:GLU:HB3  | 18       | 0.14          |
| (1,479) | 1:29:A:GLU:HA   | 1:72:A:SER:H    | 12       | 0.14          |
| (1,414) | 1:21:A:ILE:HG13 | 1:25:A:ASP:HB2  | 16       | 0.14          |
| (1,387) | 1:18:A:LEU:HB2  | 1:21:A:ILE:HG12 | 9        | 0.14          |
| (1,387) | 1:18:A:LEU:HB2  | 1:21:A:ILE:HG12 | 13       | 0.14          |
| (1,337) | 1:15:A:VAL:HB   | 1:51:A:LEU:HG   | 1        | 0.14          |
| (1,337) | 1:15:A:VAL:HB   | 1:51:A:LEU:HG   | 4        | 0.14          |
| (1,258) | 1:11:A:MET:HB2  | 1:15:A:VAL:HB   | 14       | 0.14          |
| (1,258) | 1:11:A:MET:HB2  | 1:15:A:VAL:HB   | 15       | 0.14          |
| (1,190) | 1:9:A:LYS:HA    | 1:73:A:ILE:HB   | 15       | 0.14          |
| (1,137) | 1:8:A:LEU:HA    | 1:76:A:LEU:HB2  | 12       | 0.14          |
| (1,128) | 1:8:A:LEU:HA    | 1:76:A:LEU:HB3  | 2        | 0.14          |
| (1,128) | 1:8:A:LEU:HA    | 1:76:A:LEU:HB3  | 4        | 0.14          |
| (1,128) | 1:8:A:LEU:HA    | 1:76:A:LEU:HB3  | 9        | 0.14          |
| (1,128) | 1:8:A:LEU:HA    | 1:76:A:LEU:HB3  | 12       | 0.14          |
| (1,128) | 1:8:A:LEU:HA    | 1:76:A:LEU:HB3  | 20       | 0.14          |
| (1,125) | 1:8:A:LEU:HB3   | 1:77:A:VAL:HA   | 12       | 0.14          |
| (1,125) | 1:8:A:LEU:HB3   | 1:77:A:VAL:HA   | 13       | 0.14          |
| (1,113) | 1:7:A:GLU:HA    | 1:11:A:MET:HB3  | 16       | 0.14          |
| (1,112) | 1:7:A:GLU:HB3   | 1:10:A:GLN:HB2  | 2        | 0.14          |
| (1,68)  | 1:5:A:ALA:HA    | 1:9:A:LYS:HB2   | 1        | 0.14          |
| (1,66)  | 1:5:A:ALA:HA    | 1:73:A:ILE:HG13 | 2        | 0.14          |
| (1,66)  | 1:5:A:ALA:HA    | 1:73:A:ILE:HG13 | 9        | 0.14          |
| (1,66)  | 1:5:A:ALA:HA    | 1:73:A:ILE:HG13 | 17       | 0.14          |
| (1,66)  | 1:5:A:ALA:HA    | 1:73:A:ILE:HG13 | 19       | 0.14          |
| (1,27)  | 1:4:A:LEU:HB2   | 1:84:A:GLN:HG3  | 4        | 0.14          |
| (1,27)  | 1:4:A:LEU:HB2   | 1:84:A:GLN:HG3  | 20       | 0.14          |
| (1,26)  | 1:4:A:LEU:HB3   | 1:81:A:GLU:HA   | 9        | 0.14          |
| (1,26)  | 1:4:A:LEU:HB3   | 1:81:A:GLU:HA   | 17       | 0.14          |
| (1,19)  | 1:4:A:LEU:HG    | 1:81:A:GLU:HA   | 1        | 0.14          |
| (1,19)  | 1:4:A:LEU:HG    | 1:81:A:GLU:HA   | 7        | 0.14          |
| (1,19)  | 1:4:A:LEU:HG    | 1:81:A:GLU:HA   | 14       | 0.14          |
| (1,19)  | 1:4:A:LEU:HG    | 1:81:A:GLU:HA   | 19       | 0.14          |
| (1,16)  | 1:4:A:LEU:HB2   | 1:77:A:VAL:HB   | 1        | 0.14          |
| (1,16)  | 1:4:A:LEU:HB2   | 1:77:A:VAL:HB   | 2        | 0.14          |
| (1,16)  | 1:4:A:LEU:HB2   | 1:77:A:VAL:HB   | 19       | 0.14          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,15)   | 1:4:A:LEU:HG   | 1:7:A:GLU:HB2  | 5        | 0.14          |
| (1,15)   | 1:4:A:LEU:HG   | 1:7:A:GLU:HB2  | 11       | 0.14          |
| (1,15)   | 1:4:A:LEU:HG   | 1:7:A:GLU:HB2  | 13       | 0.14          |
| (1,15)   | 1:4:A:LEU:HG   | 1:7:A:GLU:HB2  | 15       | 0.14          |
| (1,13)   | 1:4:A:LEU:HG   | 1:8:A:LEU:HA   | 7        | 0.14          |
| (1,12)   | 1:4:A:LEU:HA   | 1:7:A:GLU:HA   | 4        | 0.14          |
| (1,12)   | 1:4:A:LEU:HA   | 1:7:A:GLU:HA   | 9        | 0.14          |
| (1,12)   | 1:4:A:LEU:HA   | 1:7:A:GLU:HA   | 19       | 0.14          |
| (1,2)    | 1:2:A:SER:H    | 1:4:A:LEU:HB3  | 11       | 0.14          |
| (1,2)    | 1:2:A:SER:H    | 1:4:A:LEU:HB3  | 16       | 0.14          |
| (2,69)   | 1:77:A:VAL:O   | 1:81:A:GLU:N   | 1        | 0.13          |
| (2,69)   | 1:77:A:VAL:O   | 1:81:A:GLU:N   | 2        | 0.13          |
| (2,69)   | 1:77:A:VAL:O   | 1:81:A:GLU:N   | 4        | 0.13          |
| (2,69)   | 1:77:A:VAL:O   | 1:81:A:GLU:N   | 6        | 0.13          |
| (2,69)   | 1:77:A:VAL:O   | 1:81:A:GLU:N   | 7        | 0.13          |
| (2,69)   | 1:77:A:VAL:O   | 1:81:A:GLU:N   | 8        | 0.13          |
| (2,69)   | 1:77:A:VAL:O   | 1:81:A:GLU:N   | 10       | 0.13          |
| (2,69)   | 1:77:A:VAL:O   | 1:81:A:GLU:N   | 13       | 0.13          |
| (2,69)   | 1:77:A:VAL:O   | 1:81:A:GLU:N   | 15       | 0.13          |
| (2,69)   | 1:77:A:VAL:O   | 1:81:A:GLU:N   | 17       | 0.13          |
| (2,69)   | 1:77:A:VAL:O   | 1:81:A:GLU:N   | 18       | 0.13          |
| (2,69)   | 1:77:A:VAL:O   | 1:81:A:GLU:N   | 19       | 0.13          |
| (2,61)   | 1:73:A:ILE:O   | 1:77:A:VAL:N   | 1        | 0.13          |
| (2,61)   | 1:73:A:ILE:O   | 1:77:A:VAL:N   | 3        | 0.13          |
| (2,61)   | 1:73:A:ILE:O   | 1:77:A:VAL:N   | 4        | 0.13          |
| (2,61)   | 1:73:A:ILE:O   | 1:77:A:VAL:N   | 6        | 0.13          |
| (2,61)   | 1:73:A:ILE:O   | 1:77:A:VAL:N   | 10       | 0.13          |
| (2,61)   | 1:73:A:ILE:O   | 1:77:A:VAL:N   | 11       | 0.13          |
| (2,61)   | 1:73:A:ILE:O   | 1:77:A:VAL:N   | 15       | 0.13          |
| (2,61)   | 1:73:A:ILE:O   | 1:77:A:VAL:N   | 16       | 0.13          |
| (2,61)   | 1:73:A:ILE:O   | 1:77:A:VAL:N   | 20       | 0.13          |
| (2,51)   | 1:63:A:SER:O   | 1:67:A:LYS:H   | 5        | 0.13          |
| (2,49)   | 1:52:A:LYS:O   | 1:56:A:ASN:N   | 7        | 0.13          |
| (1,1217) | 1:83:A:GLN:H   | 1:85:A:LYS:H   | 2        | 0.13          |
| (1,1217) | 1:83:A:GLN:H   | 1:85:A:LYS:H   | 8        | 0.13          |
| (1,1175) | 1:80:A:VAL:HA  | 1:84:A:GLN:HG2 | 1        | 0.13          |
| (1,1169) | 1:80:A:VAL:HB  | 1:84:A:GLN:HG2 | 2        | 0.13          |
| (1,1168) | 1:80:A:VAL:HA  | 1:83:A:GLN:HA  | 8        | 0.13          |
| (1,1168) | 1:80:A:VAL:HA  | 1:83:A:GLN:HA  | 11       | 0.13          |
| (1,1168) | 1:80:A:VAL:HA  | 1:83:A:GLN:HA  | 12       | 0.13          |
| (1,1158) | 1:79:A:LEU:HB3 | 1:82:A:ALA:H   | 5        | 0.13          |
| (1,1158) | 1:79:A:LEU:HB3 | 1:82:A:ALA:H   | 8        | 0.13          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1158) | 1:79:A:LEU:HB3  | 1:82:A:ALA:H   | 20       | 0.13          |
| (1,1157) | 1:79:A:LEU:H    | 1:81:A:GLU:H   | 2        | 0.13          |
| (1,1157) | 1:79:A:LEU:H    | 1:81:A:GLU:H   | 6        | 0.13          |
| (1,1157) | 1:79:A:LEU:H    | 1:81:A:GLU:H   | 10       | 0.13          |
| (1,1157) | 1:79:A:LEU:H    | 1:81:A:GLU:H   | 11       | 0.13          |
| (1,1157) | 1:79:A:LEU:H    | 1:81:A:GLU:H   | 16       | 0.13          |
| (1,1157) | 1:79:A:LEU:H    | 1:81:A:GLU:H   | 18       | 0.13          |
| (1,1156) | 1:79:A:LEU:HB2  | 1:82:A:ALA:H   | 2        | 0.13          |
| (1,1156) | 1:79:A:LEU:HB2  | 1:82:A:ALA:H   | 4        | 0.13          |
| (1,1156) | 1:79:A:LEU:HB2  | 1:82:A:ALA:H   | 8        | 0.13          |
| (1,1156) | 1:79:A:LEU:HB2  | 1:82:A:ALA:H   | 11       | 0.13          |
| (1,1145) | 1:78:A:ALA:H    | 1:80:A:VAL:H   | 4        | 0.13          |
| (1,1121) | 1:77:A:VAL:HA   | 1:80:A:VAL:HA  | 20       | 0.13          |
| (1,1118) | 1:77:A:VAL:HB   | 1:81:A:GLU:H   | 12       | 0.13          |
| (1,1118) | 1:77:A:VAL:HB   | 1:81:A:GLU:H   | 20       | 0.13          |
| (1,1091) | 1:76:A:LEU:HG   | 1:79:A:LEU:HB2 | 16       | 0.13          |
| (1,1078) | 1:75:A:SER:HB2  | 1:79:A:LEU:H   | 5        | 0.13          |
| (1,1078) | 1:75:A:SER:HB2  | 1:79:A:LEU:H   | 8        | 0.13          |
| (1,1078) | 1:75:A:SER:HB2  | 1:79:A:LEU:H   | 12       | 0.13          |
| (1,1078) | 1:75:A:SER:HB2  | 1:79:A:LEU:H   | 18       | 0.13          |
| (1,1064) | 1:74:A:GLN:H    | 1:77:A:VAL:HB  | 19       | 0.13          |
| (1,1039) | 1:73:A:ILE:HB   | 1:76:A:LEU:HG  | 1        | 0.13          |
| (1,1039) | 1:73:A:ILE:HB   | 1:76:A:LEU:HG  | 16       | 0.13          |
| (1,1035) | 1:73:A:ILE:HG12 | 1:76:A:LEU:HB2 | 15       | 0.13          |
| (1,1035) | 1:73:A:ILE:HG12 | 1:76:A:LEU:HB2 | 16       | 0.13          |
| (1,986)  | 1:70:A:PHE:HB3  | 1:75:A:SER:HB2 | 2        | 0.13          |
| (1,986)  | 1:70:A:PHE:HB3  | 1:75:A:SER:HB2 | 10       | 0.13          |
| (1,986)  | 1:70:A:PHE:HB3  | 1:75:A:SER:HB2 | 11       | 0.13          |
| (1,986)  | 1:70:A:PHE:HB3  | 1:75:A:SER:HB2 | 13       | 0.13          |
| (1,986)  | 1:70:A:PHE:HB3  | 1:75:A:SER:HB2 | 14       | 0.13          |
| (1,986)  | 1:70:A:PHE:HB3  | 1:75:A:SER:HB2 | 19       | 0.13          |
| (1,985)  | 1:70:A:PHE:HB2  | 1:75:A:SER:HB2 | 10       | 0.13          |
| (1,985)  | 1:70:A:PHE:HB2  | 1:75:A:SER:HB2 | 16       | 0.13          |
| (1,963)  | 1:69:A:HIS:HA   | 1:76:A:LEU:HA  | 14       | 0.13          |
| (1,962)  | 1:69:A:HIS:HB2  | 1:76:A:LEU:HG  | 8        | 0.13          |
| (1,962)  | 1:69:A:HIS:HB2  | 1:76:A:LEU:HG  | 9        | 0.13          |
| (1,962)  | 1:69:A:HIS:HB2  | 1:76:A:LEU:HG  | 17       | 0.13          |
| (1,961)  | 1:69:A:HIS:H    | 1:75:A:SER:HB2 | 5        | 0.13          |
| (1,961)  | 1:69:A:HIS:H    | 1:75:A:SER:HB2 | 7        | 0.13          |
| (1,961)  | 1:69:A:HIS:H    | 1:75:A:SER:HB2 | 13       | 0.13          |
| (1,961)  | 1:69:A:HIS:H    | 1:75:A:SER:HB2 | 15       | 0.13          |
| (1,959)  | 1:69:A:HIS:HB2  | 1:79:A:LEU:H   | 1        | 0.13          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,959) | 1:69:A:HIS:HB2 | 1:79:A:LEU:H   | 4        | 0.13          |
| (1,959) | 1:69:A:HIS:HB2 | 1:79:A:LEU:H   | 9        | 0.13          |
| (1,941) | 1:66:A:THR:H   | 1:68:A:GLN:HG2 | 17       | 0.13          |
| (1,917) | 1:65:A:GLU:HA  | 1:68:A:GLN:HA  | 3        | 0.13          |
| (1,917) | 1:65:A:GLU:HA  | 1:68:A:GLN:HA  | 4        | 0.13          |
| (1,917) | 1:65:A:GLU:HA  | 1:68:A:GLN:HA  | 7        | 0.13          |
| (1,917) | 1:65:A:GLU:HA  | 1:68:A:GLN:HA  | 19       | 0.13          |
| (1,903) | 1:64:A:ASP:H   | 1:67:A:LYS:H   | 17       | 0.13          |
| (1,892) | 1:63:A:SER:HA  | 1:67:A:LYS:HG2 | 1        | 0.13          |
| (1,892) | 1:63:A:SER:HA  | 1:67:A:LYS:HG2 | 13       | 0.13          |
| (1,892) | 1:63:A:SER:HA  | 1:67:A:LYS:HG2 | 20       | 0.13          |
| (1,891) | 1:63:A:SER:H   | 1:65:A:GLU:H   | 5        | 0.13          |
| (1,891) | 1:63:A:SER:H   | 1:65:A:GLU:H   | 14       | 0.13          |
| (1,891) | 1:63:A:SER:H   | 1:65:A:GLU:H   | 16       | 0.13          |
| (1,886) | 1:62:A:GLU:HA  | 1:67:A:LYS:HG2 | 1        | 0.13          |
| (1,886) | 1:62:A:GLU:HA  | 1:67:A:LYS:HG2 | 13       | 0.13          |
| (1,877) | 1:61:A:ALA:HA  | 1:66:A:THR:H   | 3        | 0.13          |
| (1,877) | 1:61:A:ALA:HA  | 1:66:A:THR:H   | 17       | 0.13          |
| (1,877) | 1:61:A:ALA:HA  | 1:66:A:THR:H   | 20       | 0.13          |
| (1,859) | 1:60:A:ASN:HB2 | 1:63:A:SER:HA  | 9        | 0.13          |
| (1,858) | 1:60:A:ASN:HA  | 1:66:A:THR:H   | 1        | 0.13          |
| (1,858) | 1:60:A:ASN:HA  | 1:66:A:THR:H   | 6        | 0.13          |
| (1,858) | 1:60:A:ASN:HA  | 1:66:A:THR:H   | 17       | 0.13          |
| (1,858) | 1:60:A:ASN:HA  | 1:66:A:THR:H   | 20       | 0.13          |
| (1,857) | 1:60:A:ASN:HB2 | 1:66:A:THR:HA  | 5        | 0.13          |
| (1,833) | 1:57:A:ILE:HA  | 1:59:A:LEU:H   | 17       | 0.13          |
| (1,832) | 1:57:A:ILE:HB  | 1:59:A:LEU:HG  | 11       | 0.13          |
| (1,800) | 1:55:A:TYR:HB3 | 1:80:A:VAL:HA  | 1        | 0.13          |
| (1,796) | 1:55:A:TYR:HB2 | 1:83:A:GLN:HB3 | 10       | 0.13          |
| (1,795) | 1:55:A:TYR:HB3 | 1:57:A:ILE:HA  | 9        | 0.13          |
| (1,795) | 1:55:A:TYR:HB3 | 1:57:A:ILE:HA  | 10       | 0.13          |
| (1,794) | 1:55:A:TYR:HB2 | 1:84:A:GLN:HG2 | 7        | 0.13          |
| (1,789) | 1:54:A:ARG:H   | 1:55:A:TYR:HA  | 13       | 0.13          |
| (1,784) | 1:53:A:LYS:HA  | 1:55:A:TYR:H   | 8        | 0.13          |
| (1,759) | 1:52:A:LYS:HG2 | 1:58:A:HIS:H   | 18       | 0.13          |
| (1,758) | 1:52:A:LYS:HG3 | 1:57:A:ILE:H   | 13       | 0.13          |
| (1,758) | 1:52:A:LYS:HG3 | 1:57:A:ILE:H   | 20       | 0.13          |
| (1,739) | 1:51:A:LEU:HB3 | 1:54:A:ARG:HB3 | 18       | 0.13          |
| (1,737) | 1:51:A:LEU:HA  | 1:57:A:ILE:H   | 2        | 0.13          |
| (1,737) | 1:51:A:LEU:HA  | 1:57:A:ILE:H   | 11       | 0.13          |
| (1,737) | 1:51:A:LEU:HA  | 1:57:A:ILE:H   | 13       | 0.13          |
| (1,737) | 1:51:A:LEU:HA  | 1:57:A:ILE:H   | 15       | 0.13          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,737) | 1:51:A:LEU:HA  | 1:57:A:ILE:H   | 17       | 0.13          |
| (1,736) | 1:51:A:LEU:HB3 | 1:59:A:LEU:HG  | 10       | 0.13          |
| (1,736) | 1:51:A:LEU:HB3 | 1:59:A:LEU:HG  | 18       | 0.13          |
| (1,710) | 1:49:A:LEU:HA  | 1:52:A:LYS:HG2 | 1        | 0.13          |
| (1,710) | 1:49:A:LEU:HA  | 1:52:A:LYS:HG2 | 3        | 0.13          |
| (1,710) | 1:49:A:LEU:HA  | 1:52:A:LYS:HG2 | 4        | 0.13          |
| (1,709) | 1:49:A:LEU:HA  | 1:59:A:LEU:HG  | 2        | 0.13          |
| (1,709) | 1:49:A:LEU:HA  | 1:59:A:LEU:HG  | 6        | 0.13          |
| (1,708) | 1:49:A:LEU:HB2 | 1:52:A:LYS:H   | 15       | 0.13          |
| (1,707) | 1:49:A:LEU:HA  | 1:53:A:LYS:H   | 9        | 0.13          |
| (1,692) | 1:48:A:GLY:HA2 | 1:51:A:LEU:HA  | 3        | 0.13          |
| (1,692) | 1:48:A:GLY:HA2 | 1:51:A:LEU:HA  | 20       | 0.13          |
| (1,691) | 1:48:A:GLY:HA3 | 1:51:A:LEU:HB3 | 13       | 0.13          |
| (1,689) | 1:48:A:GLY:HA3 | 1:52:A:LYS:HB2 | 7        | 0.13          |
| (1,689) | 1:48:A:GLY:HA3 | 1:52:A:LYS:HB2 | 18       | 0.13          |
| (1,688) | 1:48:A:GLY:HA2 | 1:59:A:LEU:HB3 | 1        | 0.13          |
| (1,688) | 1:48:A:GLY:HA2 | 1:59:A:LEU:HB3 | 5        | 0.13          |
| (1,688) | 1:48:A:GLY:HA2 | 1:59:A:LEU:HB3 | 19       | 0.13          |
| (1,676) | 1:47:A:LEU:HA  | 1:49:A:LEU:H   | 14       | 0.13          |
| (1,674) | 1:47:A:LEU:HG  | 1:51:A:LEU:HB3 | 9        | 0.13          |
| (1,674) | 1:47:A:LEU:HG  | 1:51:A:LEU:HB3 | 17       | 0.13          |
| (1,673) | 1:47:A:LEU:HB3 | 1:51:A:LEU:HG  | 13       | 0.13          |
| (1,652) | 1:45:A:LEU:HA  | 1:49:A:LEU:HB3 | 19       | 0.13          |
| (1,651) | 1:45:A:LEU:HA  | 1:48:A:GLY:HA2 | 4        | 0.13          |
| (1,648) | 1:45:A:LEU:HB2 | 1:49:A:LEU:H   | 3        | 0.13          |
| (1,648) | 1:45:A:LEU:HB2 | 1:49:A:LEU:H   | 7        | 0.13          |
| (1,648) | 1:45:A:LEU:HB2 | 1:49:A:LEU:H   | 12       | 0.13          |
| (1,648) | 1:45:A:LEU:HB2 | 1:49:A:LEU:H   | 18       | 0.13          |
| (1,648) | 1:45:A:LEU:HB2 | 1:49:A:LEU:H   | 20       | 0.13          |
| (1,647) | 1:45:A:LEU:HA  | 1:49:A:LEU:HA  | 16       | 0.13          |
| (1,647) | 1:45:A:LEU:HA  | 1:49:A:LEU:HA  | 18       | 0.13          |
| (1,647) | 1:45:A:LEU:HA  | 1:49:A:LEU:HA  | 20       | 0.13          |
| (1,631) | 1:44:A:ALA:HA  | 1:47:A:LEU:HG  | 18       | 0.13          |
| (1,629) | 1:44:A:ALA:H   | 1:47:A:LEU:HB2 | 10       | 0.13          |
| (1,628) | 1:44:A:ALA:HA  | 1:48:A:GLY:HA3 | 1        | 0.13          |
| (1,628) | 1:44:A:ALA:HA  | 1:48:A:GLY:HA3 | 7        | 0.13          |
| (1,628) | 1:44:A:ALA:HA  | 1:48:A:GLY:HA3 | 13       | 0.13          |
| (1,628) | 1:44:A:ALA:HA  | 1:48:A:GLY:HA3 | 18       | 0.13          |
| (1,616) | 1:43:A:ASP:HA  | 1:46:A:GLU:HA  | 6        | 0.13          |
| (1,616) | 1:43:A:ASP:HA  | 1:46:A:GLU:HA  | 9        | 0.13          |
| (1,616) | 1:43:A:ASP:HA  | 1:46:A:GLU:HA  | 17       | 0.13          |
| (1,600) | 1:41:A:SER:HA  | 1:45:A:LEU:H   | 2        | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,600) | 1:41:A:SER:HA   | 1:45:A:LEU:H    | 12       | 0.13          |
| (1,600) | 1:41:A:SER:HA   | 1:45:A:LEU:H    | 20       | 0.13          |
| (1,572) | 1:39:A:LEU:HA   | 1:43:A:ASP:H    | 15       | 0.13          |
| (1,571) | 1:39:A:LEU:HB2  | 1:43:A:ASP:H    | 10       | 0.13          |
| (1,571) | 1:39:A:LEU:HB2  | 1:43:A:ASP:H    | 17       | 0.13          |
| (1,545) | 1:33:A:PHE:HE1  | 1:40:A:ASP:H    | 15       | 0.13          |
| (1,536) | 1:33:A:PHE:HE1  | 1:39:A:LEU:H    | 13       | 0.13          |
| (1,535) | 1:33:A:PHE:HA   | 1:39:A:LEU:HB3  | 8        | 0.13          |
| (1,505) | 1:31:A:PRO:HB3  | 1:34:A:GLY:HA2  | 13       | 0.13          |
| (1,480) | 1:29:A:GLU:H    | 1:74:A:GLN:HB3  | 2        | 0.13          |
| (1,479) | 1:29:A:GLU:HA   | 1:72:A:SER:H    | 3        | 0.13          |
| (1,479) | 1:29:A:GLU:HA   | 1:72:A:SER:H    | 5        | 0.13          |
| (1,479) | 1:29:A:GLU:HA   | 1:72:A:SER:H    | 9        | 0.13          |
| (1,479) | 1:29:A:GLU:HA   | 1:72:A:SER:H    | 20       | 0.13          |
| (1,414) | 1:21:A:ILE:HG13 | 1:25:A:ASP:HB2  | 10       | 0.13          |
| (1,414) | 1:21:A:ILE:HG13 | 1:25:A:ASP:HB2  | 14       | 0.13          |
| (1,406) | 1:19:A:GLU:HB3  | 1:21:A:ILE:H    | 1        | 0.13          |
| (1,406) | 1:19:A:GLU:HB3  | 1:21:A:ILE:H    | 5        | 0.13          |
| (1,406) | 1:19:A:GLU:HB3  | 1:21:A:ILE:H    | 12       | 0.13          |
| (1,389) | 1:18:A:LEU:HG   | 1:37:A:LEU:HB3  | 10       | 0.13          |
| (1,387) | 1:18:A:LEU:HB2  | 1:21:A:ILE:HG12 | 4        | 0.13          |
| (1,387) | 1:18:A:LEU:HB2  | 1:21:A:ILE:HG12 | 16       | 0.13          |
| (1,387) | 1:18:A:LEU:HB2  | 1:21:A:ILE:HG12 | 17       | 0.13          |
| (1,362) | 1:16:A:LEU:HG   | 1:43:A:ASP:HB2  | 16       | 0.13          |
| (1,360) | 1:16:A:LEU:HB2  | 1:37:A:LEU:HG   | 13       | 0.13          |
| (1,360) | 1:16:A:LEU:HB2  | 1:37:A:LEU:HG   | 18       | 0.13          |
| (1,360) | 1:16:A:LEU:HB2  | 1:37:A:LEU:HG   | 19       | 0.13          |
| (1,337) | 1:15:A:VAL:HB   | 1:51:A:LEU:HG   | 6        | 0.13          |
| (1,337) | 1:15:A:VAL:HB   | 1:51:A:LEU:HG   | 13       | 0.13          |
| (1,337) | 1:15:A:VAL:HB   | 1:51:A:LEU:HG   | 16       | 0.13          |
| (1,337) | 1:15:A:VAL:HB   | 1:51:A:LEU:HG   | 17       | 0.13          |
| (1,337) | 1:15:A:VAL:HB   | 1:51:A:LEU:HG   | 18       | 0.13          |
| (1,337) | 1:15:A:VAL:HB   | 1:51:A:LEU:HG   | 20       | 0.13          |
| (1,308) | 1:13:A:ILE:HA   | 1:18:A:LEU:HA   | 4        | 0.13          |
| (1,308) | 1:13:A:ILE:HA   | 1:18:A:LEU:HA   | 16       | 0.13          |
| (1,263) | 1:11:A:MET:HB3  | 1:15:A:VAL:H    | 1        | 0.13          |
| (1,263) | 1:11:A:MET:HB3  | 1:15:A:VAL:H    | 18       | 0.13          |
| (1,260) | 1:11:A:MET:HE1  | 1:15:A:VAL:HA   | 7        | 0.13          |
| (1,260) | 1:11:A:MET:HE2  | 1:15:A:VAL:HA   | 7        | 0.13          |
| (1,260) | 1:11:A:MET:HE3  | 1:15:A:VAL:HA   | 7        | 0.13          |
| (1,258) | 1:11:A:MET:HB2  | 1:15:A:VAL:HB   | 6        | 0.13          |
| (1,257) | 1:11:A:MET:HA   | 1:15:A:VAL:HA   | 6        | 0.13          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,257) | 1:11:A:MET:HA  | 1:15:A:VAL:HA   | 11       | 0.13          |
| (1,257) | 1:11:A:MET:HA  | 1:15:A:VAL:HA   | 14       | 0.13          |
| (1,257) | 1:11:A:MET:HA  | 1:15:A:VAL:HA   | 16       | 0.13          |
| (1,232) | 1:10:A:GLN:HG3 | 1:23:A:ILE:HG13 | 3        | 0.13          |
| (1,231) | 1:10:A:GLN:HA  | 1:12:A:ILE:HB   | 2        | 0.13          |
| (1,231) | 1:10:A:GLN:HA  | 1:12:A:ILE:HB   | 12       | 0.13          |
| (1,231) | 1:10:A:GLN:HA  | 1:12:A:ILE:HB   | 18       | 0.13          |
| (1,227) | 1:10:A:GLN:HG2 | 1:14:A:ASP:HA   | 2        | 0.13          |
| (1,227) | 1:10:A:GLN:HG2 | 1:14:A:ASP:HA   | 4        | 0.13          |
| (1,193) | 1:9:A:LYS:HA   | 1:26:A:ILE:HB   | 19       | 0.13          |
| (1,190) | 1:9:A:LYS:HA   | 1:73:A:ILE:HB   | 16       | 0.13          |
| (1,186) | 1:9:A:LYS:H    | 1:11:A:MET:HB2  | 7        | 0.13          |
| (1,184) | 1:9:A:LYS:HB2  | 1:13:A:ILE:HG13 | 4        | 0.13          |
| (1,184) | 1:9:A:LYS:HB2  | 1:13:A:ILE:HG13 | 19       | 0.13          |
| (1,182) | 1:9:A:LYS:HA   | 1:13:A:ILE:HB   | 15       | 0.13          |
| (1,182) | 1:9:A:LYS:HA   | 1:13:A:ILE:HB   | 19       | 0.13          |
| (1,142) | 1:8:A:LEU:HA   | 1:11:A:MET:HA   | 12       | 0.13          |
| (1,137) | 1:8:A:LEU:HA   | 1:76:A:LEU:HB2  | 2        | 0.13          |
| (1,131) | 1:8:A:LEU:HA   | 1:12:A:ILE:HG12 | 4        | 0.13          |
| (1,128) | 1:8:A:LEU:HA   | 1:76:A:LEU:HB3  | 3        | 0.13          |
| (1,128) | 1:8:A:LEU:HA   | 1:76:A:LEU:HB3  | 8        | 0.13          |
| (1,128) | 1:8:A:LEU:HA   | 1:76:A:LEU:HB3  | 17       | 0.13          |
| (1,125) | 1:8:A:LEU:HB3  | 1:77:A:VAL:HA   | 4        | 0.13          |
| (1,125) | 1:8:A:LEU:HB3  | 1:77:A:VAL:HA   | 5        | 0.13          |
| (1,125) | 1:8:A:LEU:HB3  | 1:77:A:VAL:HA   | 9        | 0.13          |
| (1,112) | 1:7:A:GLU:HB3  | 1:10:A:GLN:HB2  | 4        | 0.13          |
| (1,112) | 1:7:A:GLU:HB3  | 1:10:A:GLN:HB2  | 19       | 0.13          |
| (1,70)  | 1:5:A:ALA:H    | 1:77:A:VAL:HA   | 15       | 0.13          |
| (1,66)  | 1:5:A:ALA:HA   | 1:73:A:ILE:HG13 | 4        | 0.13          |
| (1,66)  | 1:5:A:ALA:HA   | 1:73:A:ILE:HG13 | 6        | 0.13          |
| (1,66)  | 1:5:A:ALA:HA   | 1:73:A:ILE:HG13 | 7        | 0.13          |
| (1,66)  | 1:5:A:ALA:HA   | 1:73:A:ILE:HG13 | 14       | 0.13          |
| (1,27)  | 1:4:A:LEU:HB2  | 1:84:A:GLN:HG3  | 3        | 0.13          |
| (1,27)  | 1:4:A:LEU:HB2  | 1:84:A:GLN:HG3  | 5        | 0.13          |
| (1,27)  | 1:4:A:LEU:HB2  | 1:84:A:GLN:HG3  | 9        | 0.13          |
| (1,27)  | 1:4:A:LEU:HB2  | 1:84:A:GLN:HG3  | 17       | 0.13          |
| (1,26)  | 1:4:A:LEU:HB3  | 1:81:A:GLU:HA   | 14       | 0.13          |
| (1,26)  | 1:4:A:LEU:HB3  | 1:81:A:GLU:HA   | 19       | 0.13          |
| (1,22)  | 1:4:A:LEU:HB2  | 1:77:A:VAL:HA   | 4        | 0.13          |
| (1,22)  | 1:4:A:LEU:HB2  | 1:77:A:VAL:HA   | 15       | 0.13          |
| (1,22)  | 1:4:A:LEU:HB2  | 1:77:A:VAL:HA   | 19       | 0.13          |
| (1,19)  | 1:4:A:LEU:HG   | 1:81:A:GLU:HA   | 3        | 0.13          |

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| Key    | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|--------|---------------|----------------|----------|---------------|
| (1,18) | 1:4:A:LEU:HA  | 1:8:A:LEU:HA   | 8        | 0.13          |
| (1,18) | 1:4:A:LEU:HA  | 1:8:A:LEU:HA   | 18       | 0.13          |
| (1,16) | 1:4:A:LEU:HB2 | 1:77:A:VAL:HB  | 4        | 0.13          |
| (1,16) | 1:4:A:LEU:HB2 | 1:77:A:VAL:HB  | 7        | 0.13          |
| (1,16) | 1:4:A:LEU:HB2 | 1:77:A:VAL:HB  | 16       | 0.13          |
| (1,15) | 1:4:A:LEU:HG  | 1:7:A:GLU:HB2  | 10       | 0.13          |
| (1,15) | 1:4:A:LEU:HG  | 1:7:A:GLU:HB2  | 12       | 0.13          |
| (1,15) | 1:4:A:LEU:HG  | 1:7:A:GLU:HB2  | 16       | 0.13          |
| (1,14) | 1:4:A:LEU:HB2 | 1:8:A:LEU:HB2  | 6        | 0.13          |
| (1,14) | 1:4:A:LEU:HB2 | 1:8:A:LEU:HB2  | 13       | 0.13          |
| (1,14) | 1:4:A:LEU:HB2 | 1:8:A:LEU:HB2  | 15       | 0.13          |
| (1,13) | 1:4:A:LEU:HG  | 1:8:A:LEU:HA   | 5        | 0.13          |
| (1,13) | 1:4:A:LEU:HG  | 1:8:A:LEU:HA   | 10       | 0.13          |
| (1,13) | 1:4:A:LEU:HG  | 1:8:A:LEU:HA   | 14       | 0.13          |
| (1,12) | 1:4:A:LEU:HA  | 1:7:A:GLU:HA   | 2        | 0.13          |
| (1,12) | 1:4:A:LEU:HA  | 1:7:A:GLU:HA   | 11       | 0.13          |
| (1,12) | 1:4:A:LEU:HA  | 1:7:A:GLU:HA   | 14       | 0.13          |
| (1,12) | 1:4:A:LEU:HA  | 1:7:A:GLU:HA   | 16       | 0.13          |
| (1,12) | 1:4:A:LEU:HA  | 1:7:A:GLU:HA   | 20       | 0.13          |
| (1,3)  | 1:2:A:SER:HB2 | 1:81:A:GLU:HG2 | 18       | 0.13          |
| (1,3)  | 1:2:A:SER:HB2 | 1:81:A:GLU:HG3 | 18       | 0.13          |
| (1,3)  | 1:2:A:SER:HB3 | 1:81:A:GLU:HG2 | 18       | 0.13          |
| (1,3)  | 1:2:A:SER:HB3 | 1:81:A:GLU:HG3 | 18       | 0.13          |
| (1,2)  | 1:2:A:SER:H   | 1:4:A:LEU:HB3  | 5        | 0.13          |
| (1,2)  | 1:2:A:SER:H   | 1:4:A:LEU:HB3  | 12       | 0.13          |
| (1,2)  | 1:2:A:SER:H   | 1:4:A:LEU:HB3  | 14       | 0.13          |
| (1,2)  | 1:2:A:SER:H   | 1:4:A:LEU:HB3  | 17       | 0.13          |
| (2,71) | 1:78:A:ALA:O  | 1:82:A:ALA:H   | 20       | 0.12          |
| (2,69) | 1:77:A:VAL:O  | 1:81:A:GLU:N   | 3        | 0.12          |
| (2,69) | 1:77:A:VAL:O  | 1:81:A:GLU:N   | 5        | 0.12          |
| (2,69) | 1:77:A:VAL:O  | 1:81:A:GLU:N   | 12       | 0.12          |
| (2,51) | 1:63:A:SER:O  | 1:67:A:LYS:H   | 8        | 0.12          |
| (2,49) | 1:52:A:LYS:O  | 1:56:A:ASN:N   | 1        | 0.12          |
| (2,40) | 1:47:A:LEU:O  | 1:51:A:LEU:N   | 3        | 0.12          |
| (2,14) | 1:10:A:GLN:O  | 1:14:A:ASP:N   | 1        | 0.12          |
| (2,14) | 1:10:A:GLN:O  | 1:14:A:ASP:N   | 2        | 0.12          |
| (2,14) | 1:10:A:GLN:O  | 1:14:A:ASP:N   | 3        | 0.12          |
| (2,14) | 1:10:A:GLN:O  | 1:14:A:ASP:N   | 4        | 0.12          |
| (2,14) | 1:10:A:GLN:O  | 1:14:A:ASP:N   | 5        | 0.12          |
| (2,14) | 1:10:A:GLN:O  | 1:14:A:ASP:N   | 7        | 0.12          |
| (2,14) | 1:10:A:GLN:O  | 1:14:A:ASP:N   | 8        | 0.12          |
| (2,14) | 1:10:A:GLN:O  | 1:14:A:ASP:N   | 10       | 0.12          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (2,14)   | 1:10:A:GLN:O   | 1:14:A:ASP:N   | 11       | 0.12          |
| (2,14)   | 1:10:A:GLN:O   | 1:14:A:ASP:N   | 13       | 0.12          |
| (2,14)   | 1:10:A:GLN:O   | 1:14:A:ASP:N   | 14       | 0.12          |
| (2,14)   | 1:10:A:GLN:O   | 1:14:A:ASP:N   | 15       | 0.12          |
| (2,14)   | 1:10:A:GLN:O   | 1:14:A:ASP:N   | 16       | 0.12          |
| (2,14)   | 1:10:A:GLN:O   | 1:14:A:ASP:N   | 19       | 0.12          |
| (2,14)   | 1:10:A:GLN:O   | 1:14:A:ASP:N   | 20       | 0.12          |
| (2,8)    | 1:7:A:GLU:O    | 1:11:A:MET:N   | 3        | 0.12          |
| (1,1227) | 1:84:A:GLN:H   | 1:85:A:LYS:HB2 | 13       | 0.12          |
| (1,1217) | 1:83:A:GLN:H   | 1:85:A:LYS:H   | 12       | 0.12          |
| (1,1217) | 1:83:A:GLN:H   | 1:85:A:LYS:H   | 18       | 0.12          |
| (1,1213) | 1:82:A:ALA:HA  | 1:84:A:GLN:H   | 6        | 0.12          |
| (1,1213) | 1:82:A:ALA:HA  | 1:84:A:GLN:H   | 13       | 0.12          |
| (1,1178) | 1:80:A:VAL:HA  | 1:83:A:GLN:HB2 | 5        | 0.12          |
| (1,1175) | 1:80:A:VAL:HA  | 1:84:A:GLN:HG2 | 9        | 0.12          |
| (1,1170) | 1:80:A:VAL:HB  | 1:82:A:ALA:H   | 5        | 0.12          |
| (1,1169) | 1:80:A:VAL:HB  | 1:84:A:GLN:HG2 | 11       | 0.12          |
| (1,1168) | 1:80:A:VAL:HA  | 1:83:A:GLN:HA  | 2        | 0.12          |
| (1,1158) | 1:79:A:LEU:HB3 | 1:82:A:ALA:H   | 2        | 0.12          |
| (1,1158) | 1:79:A:LEU:HB3 | 1:82:A:ALA:H   | 4        | 0.12          |
| (1,1158) | 1:79:A:LEU:HB3 | 1:82:A:ALA:H   | 7        | 0.12          |
| (1,1158) | 1:79:A:LEU:HB3 | 1:82:A:ALA:H   | 15       | 0.12          |
| (1,1158) | 1:79:A:LEU:HB3 | 1:82:A:ALA:H   | 18       | 0.12          |
| (1,1157) | 1:79:A:LEU:H   | 1:81:A:GLU:H   | 5        | 0.12          |
| (1,1157) | 1:79:A:LEU:H   | 1:81:A:GLU:H   | 8        | 0.12          |
| (1,1157) | 1:79:A:LEU:H   | 1:81:A:GLU:H   | 19       | 0.12          |
| (1,1156) | 1:79:A:LEU:HB2 | 1:82:A:ALA:H   | 10       | 0.12          |
| (1,1149) | 1:78:A:ALA:H   | 1:82:A:ALA:H   | 12       | 0.12          |
| (1,1145) | 1:78:A:ALA:H   | 1:80:A:VAL:H   | 8        | 0.12          |
| (1,1145) | 1:78:A:ALA:H   | 1:80:A:VAL:H   | 9        | 0.12          |
| (1,1145) | 1:78:A:ALA:H   | 1:80:A:VAL:H   | 11       | 0.12          |
| (1,1145) | 1:78:A:ALA:H   | 1:80:A:VAL:H   | 14       | 0.12          |
| (1,1145) | 1:78:A:ALA:H   | 1:80:A:VAL:H   | 19       | 0.12          |
| (1,1121) | 1:77:A:VAL:HA  | 1:80:A:VAL:HA  | 3        | 0.12          |
| (1,1118) | 1:77:A:VAL:HB  | 1:81:A:GLU:H   | 3        | 0.12          |
| (1,1118) | 1:77:A:VAL:HB  | 1:81:A:GLU:H   | 15       | 0.12          |
| (1,1113) | 1:77:A:VAL:HB  | 1:79:A:LEU:H   | 15       | 0.12          |
| (1,1113) | 1:77:A:VAL:HB  | 1:79:A:LEU:H   | 16       | 0.12          |
| (1,1091) | 1:76:A:LEU:HG  | 1:79:A:LEU:HB2 | 1        | 0.12          |
| (1,1091) | 1:76:A:LEU:HG  | 1:79:A:LEU:HB2 | 4        | 0.12          |
| (1,1091) | 1:76:A:LEU:HG  | 1:79:A:LEU:HB2 | 11       | 0.12          |
| (1,1091) | 1:76:A:LEU:HG  | 1:79:A:LEU:HB2 | 14       | 0.12          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1091) | 1:76:A:LEU:HG  | 1:79:A:LEU:HB2 | 19       | 0.12          |
| (1,1080) | 1:75:A:SER:HB3 | 1:79:A:LEU:HG  | 3        | 0.12          |
| (1,1080) | 1:75:A:SER:HB3 | 1:79:A:LEU:HG  | 20       | 0.12          |
| (1,1078) | 1:75:A:SER:HB2 | 1:79:A:LEU:H   | 3        | 0.12          |
| (1,1078) | 1:75:A:SER:HB2 | 1:79:A:LEU:H   | 9        | 0.12          |
| (1,1078) | 1:75:A:SER:HB2 | 1:79:A:LEU:H   | 11       | 0.12          |
| (1,1078) | 1:75:A:SER:HB2 | 1:79:A:LEU:H   | 14       | 0.12          |
| (1,1078) | 1:75:A:SER:HB2 | 1:79:A:LEU:H   | 17       | 0.12          |
| (1,1078) | 1:75:A:SER:HB2 | 1:79:A:LEU:H   | 20       | 0.12          |
| (1,1064) | 1:74:A:GLN:H   | 1:77:A:VAL:HB  | 1        | 0.12          |
| (1,1064) | 1:74:A:GLN:H   | 1:77:A:VAL:HB  | 3        | 0.12          |
| (1,1064) | 1:74:A:GLN:H   | 1:77:A:VAL:HB  | 5        | 0.12          |
| (1,1064) | 1:74:A:GLN:H   | 1:77:A:VAL:HB  | 7        | 0.12          |
| (1,1064) | 1:74:A:GLN:H   | 1:77:A:VAL:HB  | 15       | 0.12          |
| (1,1034) | 1:73:A:ILE:HB  | 1:77:A:VAL:HB  | 8        | 0.12          |
| (1,1034) | 1:73:A:ILE:HB  | 1:77:A:VAL:HB  | 10       | 0.12          |
| (1,1034) | 1:73:A:ILE:HB  | 1:77:A:VAL:HB  | 12       | 0.12          |
| (1,1034) | 1:73:A:ILE:HB  | 1:77:A:VAL:HB  | 17       | 0.12          |
| (1,1033) | 1:73:A:ILE:HA  | 1:77:A:VAL:HA  | 4        | 0.12          |
| (1,1033) | 1:73:A:ILE:HA  | 1:77:A:VAL:HA  | 8        | 0.12          |
| (1,1033) | 1:73:A:ILE:HA  | 1:77:A:VAL:HA  | 9        | 0.12          |
| (1,1033) | 1:73:A:ILE:HA  | 1:77:A:VAL:HA  | 11       | 0.12          |
| (1,1033) | 1:73:A:ILE:HA  | 1:77:A:VAL:HA  | 12       | 0.12          |
| (1,1033) | 1:73:A:ILE:HA  | 1:77:A:VAL:HA  | 13       | 0.12          |
| (1,1032) | 1:73:A:ILE:H   | 1:76:A:LEU:HG  | 2        | 0.12          |
| (1,1032) | 1:73:A:ILE:H   | 1:76:A:LEU:HG  | 8        | 0.12          |
| (1,1032) | 1:73:A:ILE:H   | 1:76:A:LEU:HG  | 11       | 0.12          |
| (1,1032) | 1:73:A:ILE:H   | 1:76:A:LEU:HG  | 18       | 0.12          |
| (1,986)  | 1:70:A:PHE:HB3 | 1:75:A:SER:HB2 | 4        | 0.12          |
| (1,986)  | 1:70:A:PHE:HB3 | 1:75:A:SER:HB2 | 7        | 0.12          |
| (1,986)  | 1:70:A:PHE:HB3 | 1:75:A:SER:HB2 | 8        | 0.12          |
| (1,986)  | 1:70:A:PHE:HB3 | 1:75:A:SER:HB2 | 15       | 0.12          |
| (1,986)  | 1:70:A:PHE:HB3 | 1:75:A:SER:HB2 | 18       | 0.12          |
| (1,985)  | 1:70:A:PHE:HB2 | 1:75:A:SER:HB2 | 2        | 0.12          |
| (1,985)  | 1:70:A:PHE:HB2 | 1:75:A:SER:HB2 | 11       | 0.12          |
| (1,985)  | 1:70:A:PHE:HB2 | 1:75:A:SER:HB2 | 13       | 0.12          |
| (1,985)  | 1:70:A:PHE:HB2 | 1:75:A:SER:HB2 | 14       | 0.12          |
| (1,985)  | 1:70:A:PHE:HB2 | 1:75:A:SER:HB2 | 18       | 0.12          |
| (1,962)  | 1:69:A:HIS:HB2 | 1:76:A:LEU:HG  | 2        | 0.12          |
| (1,962)  | 1:69:A:HIS:HB2 | 1:76:A:LEU:HG  | 4        | 0.12          |
| (1,962)  | 1:69:A:HIS:HB2 | 1:76:A:LEU:HG  | 11       | 0.12          |
| (1,962)  | 1:69:A:HIS:HB2 | 1:76:A:LEU:HG  | 14       | 0.12          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,962) | 1:69:A:HIS:HB2 | 1:76:A:LEU:HG  | 19       | 0.12          |
| (1,961) | 1:69:A:HIS:H   | 1:75:A:SER:HB2 | 6        | 0.12          |
| (1,961) | 1:69:A:HIS:H   | 1:75:A:SER:HB2 | 11       | 0.12          |
| (1,951) | 1:67:A:LYS:HA  | 1:71:A:LYS:H   | 13       | 0.12          |
| (1,942) | 1:66:A:THR:HB  | 1:68:A:GLN:H   | 1        | 0.12          |
| (1,942) | 1:66:A:THR:HB  | 1:68:A:GLN:H   | 4        | 0.12          |
| (1,942) | 1:66:A:THR:HB  | 1:68:A:GLN:H   | 15       | 0.12          |
| (1,938) | 1:66:A:THR:H   | 1:69:A:HIS:H   | 2        | 0.12          |
| (1,938) | 1:66:A:THR:H   | 1:69:A:HIS:H   | 10       | 0.12          |
| (1,938) | 1:66:A:THR:H   | 1:69:A:HIS:H   | 11       | 0.12          |
| (1,917) | 1:65:A:GLU:HA  | 1:68:A:GLN:HA  | 1        | 0.12          |
| (1,917) | 1:65:A:GLU:HA  | 1:68:A:GLN:HA  | 2        | 0.12          |
| (1,917) | 1:65:A:GLU:HA  | 1:68:A:GLN:HA  | 8        | 0.12          |
| (1,917) | 1:65:A:GLU:HA  | 1:68:A:GLN:HA  | 12       | 0.12          |
| (1,917) | 1:65:A:GLU:HA  | 1:68:A:GLN:HA  | 14       | 0.12          |
| (1,917) | 1:65:A:GLU:HA  | 1:68:A:GLN:HA  | 15       | 0.12          |
| (1,917) | 1:65:A:GLU:HA  | 1:68:A:GLN:HA  | 16       | 0.12          |
| (1,917) | 1:65:A:GLU:HA  | 1:68:A:GLN:HA  | 18       | 0.12          |
| (1,917) | 1:65:A:GLU:HA  | 1:68:A:GLN:HA  | 20       | 0.12          |
| (1,897) | 1:64:A:ASP:H   | 1:68:A:GLN:H   | 3        | 0.12          |
| (1,897) | 1:64:A:ASP:H   | 1:68:A:GLN:H   | 15       | 0.12          |
| (1,892) | 1:63:A:SER:HA  | 1:67:A:LYS:HG2 | 8        | 0.12          |
| (1,892) | 1:63:A:SER:HA  | 1:67:A:LYS:HG2 | 12       | 0.12          |
| (1,892) | 1:63:A:SER:HA  | 1:67:A:LYS:HG2 | 15       | 0.12          |
| (1,892) | 1:63:A:SER:HA  | 1:67:A:LYS:HG2 | 17       | 0.12          |
| (1,892) | 1:63:A:SER:HA  | 1:67:A:LYS:HG2 | 18       | 0.12          |
| (1,891) | 1:63:A:SER:H   | 1:65:A:GLU:H   | 4        | 0.12          |
| (1,891) | 1:63:A:SER:H   | 1:65:A:GLU:H   | 9        | 0.12          |
| (1,891) | 1:63:A:SER:H   | 1:65:A:GLU:H   | 15       | 0.12          |
| (1,891) | 1:63:A:SER:H   | 1:65:A:GLU:H   | 18       | 0.12          |
| (1,886) | 1:62:A:GLU:HA  | 1:67:A:LYS:HG2 | 5        | 0.12          |
| (1,886) | 1:62:A:GLU:HA  | 1:67:A:LYS:HG2 | 6        | 0.12          |
| (1,886) | 1:62:A:GLU:HA  | 1:67:A:LYS:HG2 | 11       | 0.12          |
| (1,886) | 1:62:A:GLU:HA  | 1:67:A:LYS:HG2 | 16       | 0.12          |
| (1,877) | 1:61:A:ALA:HA  | 1:66:A:THR:H   | 1        | 0.12          |
| (1,877) | 1:61:A:ALA:HA  | 1:66:A:THR:H   | 2        | 0.12          |
| (1,877) | 1:61:A:ALA:HA  | 1:66:A:THR:H   | 8        | 0.12          |
| (1,877) | 1:61:A:ALA:HA  | 1:66:A:THR:H   | 9        | 0.12          |
| (1,859) | 1:60:A:ASN:HB2 | 1:63:A:SER:HA  | 17       | 0.12          |
| (1,858) | 1:60:A:ASN:HA  | 1:66:A:THR:H   | 9        | 0.12          |
| (1,858) | 1:60:A:ASN:HA  | 1:66:A:THR:H   | 13       | 0.12          |
| (1,857) | 1:60:A:ASN:HB2 | 1:66:A:THR:HA  | 2        | 0.12          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,857) | 1:60:A:ASN:HB2 | 1:66:A:THR:HA   | 7        | 0.12          |
| (1,850) | 1:59:A:LEU:HB2 | 1:61:A:ALA:HA   | 17       | 0.12          |
| (1,833) | 1:57:A:ILE:HA  | 1:59:A:LEU:H    | 6        | 0.12          |
| (1,833) | 1:57:A:ILE:HA  | 1:59:A:LEU:H    | 16       | 0.12          |
| (1,832) | 1:57:A:ILE:HB  | 1:59:A:LEU:HG   | 2        | 0.12          |
| (1,829) | 1:57:A:ILE:HA  | 1:80:A:VAL:HA   | 9        | 0.12          |
| (1,800) | 1:55:A:TYR:HB3 | 1:80:A:VAL:HA   | 3        | 0.12          |
| (1,800) | 1:55:A:TYR:HB3 | 1:80:A:VAL:HA   | 7        | 0.12          |
| (1,800) | 1:55:A:TYR:HB3 | 1:80:A:VAL:HA   | 14       | 0.12          |
| (1,797) | 1:55:A:TYR:HB2 | 1:57:A:ILE:HG12 | 13       | 0.12          |
| (1,797) | 1:55:A:TYR:HB2 | 1:57:A:ILE:HG13 | 13       | 0.12          |
| (1,796) | 1:55:A:TYR:HB2 | 1:83:A:GLN:HB3  | 1        | 0.12          |
| (1,796) | 1:55:A:TYR:HB2 | 1:83:A:GLN:HB3  | 7        | 0.12          |
| (1,795) | 1:55:A:TYR:HB3 | 1:57:A:ILE:HA   | 1        | 0.12          |
| (1,795) | 1:55:A:TYR:HB3 | 1:57:A:ILE:HA   | 3        | 0.12          |
| (1,795) | 1:55:A:TYR:HB3 | 1:57:A:ILE:HA   | 7        | 0.12          |
| (1,795) | 1:55:A:TYR:HB3 | 1:57:A:ILE:HA   | 13       | 0.12          |
| (1,795) | 1:55:A:TYR:HB3 | 1:57:A:ILE:HA   | 16       | 0.12          |
| (1,794) | 1:55:A:TYR:HB2 | 1:84:A:GLN:HG2  | 19       | 0.12          |
| (1,789) | 1:54:A:ARG:H   | 1:55:A:TYR:HA   | 9        | 0.12          |
| (1,784) | 1:53:A:LYS:HA  | 1:55:A:TYR:H    | 5        | 0.12          |
| (1,784) | 1:53:A:LYS:HA  | 1:55:A:TYR:H    | 11       | 0.12          |
| (1,784) | 1:53:A:LYS:HA  | 1:55:A:TYR:H    | 12       | 0.12          |
| (1,761) | 1:52:A:LYS:HA  | 1:56:A:ASN:HB3  | 9        | 0.12          |
| (1,760) | 1:52:A:LYS:HA  | 1:56:A:ASN:HB2  | 2        | 0.12          |
| (1,760) | 1:52:A:LYS:HA  | 1:56:A:ASN:HB2  | 8        | 0.12          |
| (1,760) | 1:52:A:LYS:HA  | 1:56:A:ASN:HB2  | 11       | 0.12          |
| (1,760) | 1:52:A:LYS:HA  | 1:56:A:ASN:HB2  | 12       | 0.12          |
| (1,760) | 1:52:A:LYS:HA  | 1:56:A:ASN:HB2  | 16       | 0.12          |
| (1,758) | 1:52:A:LYS:HG3 | 1:57:A:ILE:H    | 1        | 0.12          |
| (1,758) | 1:52:A:LYS:HG3 | 1:57:A:ILE:H    | 3        | 0.12          |
| (1,758) | 1:52:A:LYS:HG3 | 1:57:A:ILE:H    | 4        | 0.12          |
| (1,758) | 1:52:A:LYS:HG3 | 1:57:A:ILE:H    | 7        | 0.12          |
| (1,758) | 1:52:A:LYS:HG3 | 1:57:A:ILE:H    | 8        | 0.12          |
| (1,758) | 1:52:A:LYS:HG3 | 1:57:A:ILE:H    | 12       | 0.12          |
| (1,758) | 1:52:A:LYS:HG3 | 1:57:A:ILE:H    | 16       | 0.12          |
| (1,758) | 1:52:A:LYS:HG3 | 1:57:A:ILE:H    | 18       | 0.12          |
| (1,758) | 1:52:A:LYS:HG3 | 1:57:A:ILE:H    | 19       | 0.12          |
| (1,740) | 1:51:A:LEU:H   | 1:52:A:LYS:HB3  | 15       | 0.12          |
| (1,737) | 1:51:A:LEU:HA  | 1:57:A:ILE:H    | 12       | 0.12          |
| (1,736) | 1:51:A:LEU:HB3 | 1:59:A:LEU:HG   | 8        | 0.12          |
| (1,723) | 1:50:A:ALA:H   | 1:51:A:LEU:HA   | 13       | 0.12          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,723) | 1:50:A:ALA:H   | 1:51:A:LEU:HA  | 19       | 0.12          |
| (1,722) | 1:50:A:ALA:HA  | 1:52:A:LYS:HB3 | 10       | 0.12          |
| (1,722) | 1:50:A:ALA:HA  | 1:52:A:LYS:HB3 | 14       | 0.12          |
| (1,722) | 1:50:A:ALA:HA  | 1:52:A:LYS:HB3 | 16       | 0.12          |
| (1,722) | 1:50:A:ALA:HA  | 1:52:A:LYS:HB3 | 18       | 0.12          |
| (1,722) | 1:50:A:ALA:HA  | 1:52:A:LYS:HB3 | 19       | 0.12          |
| (1,710) | 1:49:A:LEU:HA  | 1:52:A:LYS:HG2 | 7        | 0.12          |
| (1,710) | 1:49:A:LEU:HA  | 1:52:A:LYS:HG2 | 10       | 0.12          |
| (1,710) | 1:49:A:LEU:HA  | 1:52:A:LYS:HG2 | 16       | 0.12          |
| (1,710) | 1:49:A:LEU:HA  | 1:52:A:LYS:HG2 | 19       | 0.12          |
| (1,709) | 1:49:A:LEU:HA  | 1:59:A:LEU:HG  | 8        | 0.12          |
| (1,709) | 1:49:A:LEU:HA  | 1:59:A:LEU:HG  | 13       | 0.12          |
| (1,709) | 1:49:A:LEU:HA  | 1:59:A:LEU:HG  | 16       | 0.12          |
| (1,708) | 1:49:A:LEU:HB2 | 1:52:A:LYS:H   | 3        | 0.12          |
| (1,708) | 1:49:A:LEU:HB2 | 1:52:A:LYS:H   | 4        | 0.12          |
| (1,708) | 1:49:A:LEU:HB2 | 1:52:A:LYS:H   | 10       | 0.12          |
| (1,708) | 1:49:A:LEU:HB2 | 1:52:A:LYS:H   | 14       | 0.12          |
| (1,708) | 1:49:A:LEU:HB2 | 1:52:A:LYS:H   | 16       | 0.12          |
| (1,708) | 1:49:A:LEU:HB2 | 1:52:A:LYS:H   | 20       | 0.12          |
| (1,707) | 1:49:A:LEU:HA  | 1:53:A:LYS:H   | 1        | 0.12          |
| (1,707) | 1:49:A:LEU:HA  | 1:53:A:LYS:H   | 5        | 0.12          |
| (1,707) | 1:49:A:LEU:HA  | 1:53:A:LYS:H   | 11       | 0.12          |
| (1,693) | 1:48:A:GLY:HA3 | 1:51:A:LEU:HG  | 3        | 0.12          |
| (1,693) | 1:48:A:GLY:HA3 | 1:51:A:LEU:HG  | 14       | 0.12          |
| (1,693) | 1:48:A:GLY:HA3 | 1:51:A:LEU:HG  | 19       | 0.12          |
| (1,693) | 1:48:A:GLY:HA3 | 1:51:A:LEU:HG  | 20       | 0.12          |
| (1,692) | 1:48:A:GLY:HA2 | 1:51:A:LEU:HA  | 1        | 0.12          |
| (1,692) | 1:48:A:GLY:HA2 | 1:51:A:LEU:HA  | 4        | 0.12          |
| (1,692) | 1:48:A:GLY:HA2 | 1:51:A:LEU:HA  | 7        | 0.12          |
| (1,692) | 1:48:A:GLY:HA2 | 1:51:A:LEU:HA  | 14       | 0.12          |
| (1,692) | 1:48:A:GLY:HA2 | 1:51:A:LEU:HA  | 19       | 0.12          |
| (1,691) | 1:48:A:GLY:HA3 | 1:51:A:LEU:HB3 | 6        | 0.12          |
| (1,691) | 1:48:A:GLY:HA3 | 1:51:A:LEU:HB3 | 11       | 0.12          |
| (1,691) | 1:48:A:GLY:HA3 | 1:51:A:LEU:HB3 | 18       | 0.12          |
| (1,689) | 1:48:A:GLY:HA3 | 1:52:A:LYS:HB2 | 6        | 0.12          |
| (1,689) | 1:48:A:GLY:HA3 | 1:52:A:LYS:HB2 | 8        | 0.12          |
| (1,689) | 1:48:A:GLY:HA3 | 1:52:A:LYS:HB2 | 12       | 0.12          |
| (1,689) | 1:48:A:GLY:HA3 | 1:52:A:LYS:HB2 | 13       | 0.12          |
| (1,689) | 1:48:A:GLY:HA3 | 1:52:A:LYS:HB2 | 19       | 0.12          |
| (1,688) | 1:48:A:GLY:HA2 | 1:59:A:LEU:HB3 | 4        | 0.12          |
| (1,688) | 1:48:A:GLY:HA2 | 1:59:A:LEU:HB3 | 6        | 0.12          |
| (1,688) | 1:48:A:GLY:HA2 | 1:59:A:LEU:HB3 | 8        | 0.12          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,688) | 1:48:A:GLY:HA2 | 1:59:A:LEU:HB3 | 18       | 0.12          |
| (1,687) | 1:48:A:GLY:HA2 | 1:59:A:LEU:HB2 | 7        | 0.12          |
| (1,687) | 1:48:A:GLY:HA2 | 1:59:A:LEU:HB2 | 14       | 0.12          |
| (1,687) | 1:48:A:GLY:HA2 | 1:59:A:LEU:HB2 | 19       | 0.12          |
| (1,687) | 1:48:A:GLY:HA2 | 1:59:A:LEU:HB2 | 20       | 0.12          |
| (1,676) | 1:47:A:LEU:HA  | 1:49:A:LEU:H   | 9        | 0.12          |
| (1,675) | 1:47:A:LEU:HA  | 1:51:A:LEU:HA  | 2        | 0.12          |
| (1,675) | 1:47:A:LEU:HA  | 1:51:A:LEU:HA  | 11       | 0.12          |
| (1,675) | 1:47:A:LEU:HA  | 1:51:A:LEU:HA  | 12       | 0.12          |
| (1,675) | 1:47:A:LEU:HA  | 1:51:A:LEU:HA  | 13       | 0.12          |
| (1,675) | 1:47:A:LEU:HA  | 1:51:A:LEU:HA  | 17       | 0.12          |
| (1,674) | 1:47:A:LEU:HG  | 1:51:A:LEU:HB3 | 5        | 0.12          |
| (1,674) | 1:47:A:LEU:HG  | 1:51:A:LEU:HB3 | 12       | 0.12          |
| (1,673) | 1:47:A:LEU:HB3 | 1:51:A:LEU:HG  | 5        | 0.12          |
| (1,673) | 1:47:A:LEU:HB3 | 1:51:A:LEU:HG  | 6        | 0.12          |
| (1,673) | 1:47:A:LEU:HB3 | 1:51:A:LEU:HG  | 7        | 0.12          |
| (1,673) | 1:47:A:LEU:HB3 | 1:51:A:LEU:HG  | 11       | 0.12          |
| (1,673) | 1:47:A:LEU:HB3 | 1:51:A:LEU:HG  | 12       | 0.12          |
| (1,673) | 1:47:A:LEU:HB3 | 1:51:A:LEU:HG  | 18       | 0.12          |
| (1,652) | 1:45:A:LEU:HA  | 1:49:A:LEU:HB3 | 2        | 0.12          |
| (1,652) | 1:45:A:LEU:HA  | 1:49:A:LEU:HB3 | 8        | 0.12          |
| (1,652) | 1:45:A:LEU:HA  | 1:49:A:LEU:HB3 | 16       | 0.12          |
| (1,651) | 1:45:A:LEU:HA  | 1:48:A:GLY:HA2 | 5        | 0.12          |
| (1,651) | 1:45:A:LEU:HA  | 1:48:A:GLY:HA2 | 6        | 0.12          |
| (1,651) | 1:45:A:LEU:HA  | 1:48:A:GLY:HA2 | 18       | 0.12          |
| (1,651) | 1:45:A:LEU:HA  | 1:48:A:GLY:HA2 | 19       | 0.12          |
| (1,648) | 1:45:A:LEU:HB2 | 1:49:A:LEU:H   | 6        | 0.12          |
| (1,647) | 1:45:A:LEU:HA  | 1:49:A:LEU:HA  | 11       | 0.12          |
| (1,631) | 1:44:A:ALA:HA  | 1:47:A:LEU:HG  | 3        | 0.12          |
| (1,631) | 1:44:A:ALA:HA  | 1:47:A:LEU:HG  | 12       | 0.12          |
| (1,631) | 1:44:A:ALA:HA  | 1:47:A:LEU:HG  | 13       | 0.12          |
| (1,631) | 1:44:A:ALA:HA  | 1:47:A:LEU:HG  | 20       | 0.12          |
| (1,629) | 1:44:A:ALA:H   | 1:47:A:LEU:HB2 | 4        | 0.12          |
| (1,629) | 1:44:A:ALA:H   | 1:47:A:LEU:HB2 | 12       | 0.12          |
| (1,629) | 1:44:A:ALA:H   | 1:47:A:LEU:HB2 | 18       | 0.12          |
| (1,628) | 1:44:A:ALA:HA  | 1:48:A:GLY:HA3 | 12       | 0.12          |
| (1,628) | 1:44:A:ALA:HA  | 1:48:A:GLY:HA3 | 14       | 0.12          |
| (1,628) | 1:44:A:ALA:HA  | 1:48:A:GLY:HA3 | 16       | 0.12          |
| (1,628) | 1:44:A:ALA:HA  | 1:48:A:GLY:HA3 | 20       | 0.12          |
| (1,618) | 1:43:A:ASP:HB3 | 1:46:A:GLU:H   | 3        | 0.12          |
| (1,618) | 1:43:A:ASP:HB3 | 1:46:A:GLU:H   | 11       | 0.12          |
| (1,616) | 1:43:A:ASP:HA  | 1:46:A:GLU:HA  | 11       | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,600) | 1:41:A:SER:HA   | 1:45:A:LEU:H    | 4        | 0.12          |
| (1,600) | 1:41:A:SER:HA   | 1:45:A:LEU:H    | 7        | 0.12          |
| (1,600) | 1:41:A:SER:HA   | 1:45:A:LEU:H    | 10       | 0.12          |
| (1,600) | 1:41:A:SER:HA   | 1:45:A:LEU:H    | 18       | 0.12          |
| (1,572) | 1:39:A:LEU:HA   | 1:43:A:ASP:H    | 3        | 0.12          |
| (1,572) | 1:39:A:LEU:HA   | 1:43:A:ASP:H    | 17       | 0.12          |
| (1,571) | 1:39:A:LEU:HB2  | 1:43:A:ASP:H    | 20       | 0.12          |
| (1,559) | 1:37:A:LEU:HB2  | 1:39:A:LEU:HA   | 1        | 0.12          |
| (1,559) | 1:37:A:LEU:HB2  | 1:39:A:LEU:HA   | 5        | 0.12          |
| (1,545) | 1:33:A:PHE:HE1  | 1:40:A:ASP:H    | 14       | 0.12          |
| (1,517) | 1:32:A:LEU:HB2  | 1:39:A:LEU:H    | 1        | 0.12          |
| (1,517) | 1:32:A:LEU:HB2  | 1:39:A:LEU:H    | 10       | 0.12          |
| (1,517) | 1:32:A:LEU:HB2  | 1:39:A:LEU:H    | 13       | 0.12          |
| (1,503) | 1:31:A:PRO:HB2  | 1:35:A:GLU:HB3  | 2        | 0.12          |
| (1,482) | 1:29:A:GLU:H    | 1:74:A:GLN:H    | 15       | 0.12          |
| (1,480) | 1:29:A:GLU:H    | 1:74:A:GLN:HB3  | 15       | 0.12          |
| (1,480) | 1:29:A:GLU:H    | 1:74:A:GLN:HB3  | 19       | 0.12          |
| (1,479) | 1:29:A:GLU:HA   | 1:72:A:SER:H    | 11       | 0.12          |
| (1,479) | 1:29:A:GLU:HA   | 1:72:A:SER:H    | 13       | 0.12          |
| (1,479) | 1:29:A:GLU:HA   | 1:72:A:SER:H    | 17       | 0.12          |
| (1,479) | 1:29:A:GLU:HA   | 1:72:A:SER:H    | 19       | 0.12          |
| (1,414) | 1:21:A:ILE:HG13 | 1:25:A:ASP:HB2  | 3        | 0.12          |
| (1,414) | 1:21:A:ILE:HG13 | 1:25:A:ASP:HB2  | 8        | 0.12          |
| (1,414) | 1:21:A:ILE:HG13 | 1:25:A:ASP:HB2  | 20       | 0.12          |
| (1,406) | 1:19:A:GLU:HB3  | 1:21:A:ILE:H    | 4        | 0.12          |
| (1,406) | 1:19:A:GLU:HB3  | 1:21:A:ILE:H    | 18       | 0.12          |
| (1,387) | 1:18:A:LEU:HB2  | 1:21:A:ILE:HG12 | 1        | 0.12          |
| (1,387) | 1:18:A:LEU:HB2  | 1:21:A:ILE:HG12 | 2        | 0.12          |
| (1,387) | 1:18:A:LEU:HB2  | 1:21:A:ILE:HG12 | 3        | 0.12          |
| (1,387) | 1:18:A:LEU:HB2  | 1:21:A:ILE:HG12 | 5        | 0.12          |
| (1,387) | 1:18:A:LEU:HB2  | 1:21:A:ILE:HG12 | 6        | 0.12          |
| (1,387) | 1:18:A:LEU:HB2  | 1:21:A:ILE:HG12 | 12       | 0.12          |
| (1,387) | 1:18:A:LEU:HB2  | 1:21:A:ILE:HG12 | 15       | 0.12          |
| (1,387) | 1:18:A:LEU:HB2  | 1:21:A:ILE:HG12 | 20       | 0.12          |
| (1,362) | 1:16:A:LEU:HG   | 1:43:A:ASP:HB2  | 6        | 0.12          |
| (1,362) | 1:16:A:LEU:HG   | 1:43:A:ASP:HB2  | 10       | 0.12          |
| (1,362) | 1:16:A:LEU:HG   | 1:43:A:ASP:HB2  | 17       | 0.12          |
| (1,362) | 1:16:A:LEU:HG   | 1:43:A:ASP:HB2  | 18       | 0.12          |
| (1,360) | 1:16:A:LEU:HB2  | 1:37:A:LEU:HG   | 8        | 0.12          |
| (1,357) | 1:16:A:LEU:HB2  | 1:18:A:LEU:HA   | 20       | 0.12          |
| (1,308) | 1:13:A:ILE:HA   | 1:18:A:LEU:HA   | 3        | 0.12          |
| (1,308) | 1:13:A:ILE:HA   | 1:18:A:LEU:HA   | 6        | 0.12          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,308) | 1:13:A:ILE:HA  | 1:18:A:LEU:HA   | 12       | 0.12          |
| (1,308) | 1:13:A:ILE:HA  | 1:18:A:LEU:HA   | 15       | 0.12          |
| (1,308) | 1:13:A:ILE:HA  | 1:18:A:LEU:HA   | 20       | 0.12          |
| (1,263) | 1:11:A:MET:HB3 | 1:15:A:VAL:H    | 3        | 0.12          |
| (1,263) | 1:11:A:MET:HB3 | 1:15:A:VAL:H    | 11       | 0.12          |
| (1,257) | 1:11:A:MET:HA  | 1:15:A:VAL:HA   | 1        | 0.12          |
| (1,257) | 1:11:A:MET:HA  | 1:15:A:VAL:HA   | 8        | 0.12          |
| (1,257) | 1:11:A:MET:HA  | 1:15:A:VAL:HA   | 15       | 0.12          |
| (1,257) | 1:11:A:MET:HA  | 1:15:A:VAL:HA   | 18       | 0.12          |
| (1,232) | 1:10:A:GLN:HG3 | 1:23:A:ILE:HG13 | 10       | 0.12          |
| (1,232) | 1:10:A:GLN:HG3 | 1:23:A:ILE:HG13 | 11       | 0.12          |
| (1,232) | 1:10:A:GLN:HG3 | 1:23:A:ILE:HG13 | 14       | 0.12          |
| (1,231) | 1:10:A:GLN:HA  | 1:12:A:ILE:HB   | 1        | 0.12          |
| (1,231) | 1:10:A:GLN:HA  | 1:12:A:ILE:HB   | 7        | 0.12          |
| (1,228) | 1:10:A:GLN:HG3 | 1:22:A:THR:HA   | 12       | 0.12          |
| (1,228) | 1:10:A:GLN:HG3 | 1:22:A:THR:HA   | 19       | 0.12          |
| (1,227) | 1:10:A:GLN:HG2 | 1:14:A:ASP:HA   | 8        | 0.12          |
| (1,227) | 1:10:A:GLN:HG2 | 1:14:A:ASP:HA   | 11       | 0.12          |
| (1,227) | 1:10:A:GLN:HG2 | 1:14:A:ASP:HA   | 13       | 0.12          |
| (1,227) | 1:10:A:GLN:HG2 | 1:14:A:ASP:HA   | 14       | 0.12          |
| (1,227) | 1:10:A:GLN:HG2 | 1:14:A:ASP:HA   | 17       | 0.12          |
| (1,225) | 1:10:A:GLN:HA  | 1:13:A:ILE:HA   | 2        | 0.12          |
| (1,225) | 1:10:A:GLN:HA  | 1:13:A:ILE:HA   | 6        | 0.12          |
| (1,225) | 1:10:A:GLN:HA  | 1:13:A:ILE:HA   | 9        | 0.12          |
| (1,225) | 1:10:A:GLN:HA  | 1:13:A:ILE:HA   | 11       | 0.12          |
| (1,225) | 1:10:A:GLN:HA  | 1:13:A:ILE:HA   | 13       | 0.12          |
| (1,225) | 1:10:A:GLN:HA  | 1:13:A:ILE:HA   | 15       | 0.12          |
| (1,225) | 1:10:A:GLN:HA  | 1:13:A:ILE:HA   | 16       | 0.12          |
| (1,225) | 1:10:A:GLN:HA  | 1:13:A:ILE:HA   | 18       | 0.12          |
| (1,223) | 1:10:A:GLN:HB2 | 1:22:A:THR:HB   | 1        | 0.12          |
| (1,223) | 1:10:A:GLN:HB2 | 1:22:A:THR:HB   | 4        | 0.12          |
| (1,223) | 1:10:A:GLN:HB2 | 1:22:A:THR:HB   | 5        | 0.12          |
| (1,223) | 1:10:A:GLN:HB2 | 1:22:A:THR:HB   | 8        | 0.12          |
| (1,223) | 1:10:A:GLN:HB2 | 1:22:A:THR:HB   | 14       | 0.12          |
| (1,190) | 1:9:A:LYS:HA   | 1:73:A:ILE:HB   | 3        | 0.12          |
| (1,189) | 1:9:A:LYS:HB3  | 1:26:A:ILE:HD11 | 15       | 0.12          |
| (1,189) | 1:9:A:LYS:HB3  | 1:26:A:ILE:HD12 | 15       | 0.12          |
| (1,189) | 1:9:A:LYS:HB3  | 1:26:A:ILE:HD13 | 15       | 0.12          |
| (1,187) | 1:9:A:LYS:H    | 1:12:A:ILE:HB   | 1        | 0.12          |
| (1,187) | 1:9:A:LYS:H    | 1:12:A:ILE:HB   | 12       | 0.12          |
| (1,186) | 1:9:A:LYS:H    | 1:11:A:MET:HB2  | 1        | 0.12          |
| (1,186) | 1:9:A:LYS:H    | 1:11:A:MET:HB2  | 12       | 0.12          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,186) | 1:9:A:LYS:H   | 1:11:A:MET:HB2  | 15       | 0.12          |
| (1,185) | 1:9:A:LYS:HB3 | 1:12:A:ILE:H    | 2        | 0.12          |
| (1,185) | 1:9:A:LYS:HB3 | 1:12:A:ILE:H    | 15       | 0.12          |
| (1,185) | 1:9:A:LYS:HB3 | 1:12:A:ILE:H    | 19       | 0.12          |
| (1,184) | 1:9:A:LYS:HB2 | 1:13:A:ILE:HG13 | 2        | 0.12          |
| (1,184) | 1:9:A:LYS:HB2 | 1:13:A:ILE:HG13 | 5        | 0.12          |
| (1,183) | 1:9:A:LYS:HB2 | 1:13:A:ILE:H    | 5        | 0.12          |
| (1,183) | 1:9:A:LYS:HB2 | 1:13:A:ILE:H    | 14       | 0.12          |
| (1,182) | 1:9:A:LYS:HA  | 1:13:A:ILE:HB   | 2        | 0.12          |
| (1,182) | 1:9:A:LYS:HA  | 1:13:A:ILE:HB   | 14       | 0.12          |
| (1,143) | 1:8:A:LEU:HA  | 1:12:A:ILE:HA   | 13       | 0.12          |
| (1,142) | 1:8:A:LEU:HA  | 1:11:A:MET:HA   | 2        | 0.12          |
| (1,142) | 1:8:A:LEU:HA  | 1:11:A:MET:HA   | 5        | 0.12          |
| (1,142) | 1:8:A:LEU:HA  | 1:11:A:MET:HA   | 9        | 0.12          |
| (1,137) | 1:8:A:LEU:HA  | 1:76:A:LEU:HB2  | 3        | 0.12          |
| (1,137) | 1:8:A:LEU:HA  | 1:76:A:LEU:HB2  | 4        | 0.12          |
| (1,136) | 1:8:A:LEU:HB3 | 1:12:A:ILE:HA   | 7        | 0.12          |
| (1,136) | 1:8:A:LEU:HB3 | 1:12:A:ILE:HA   | 9        | 0.12          |
| (1,136) | 1:8:A:LEU:HB3 | 1:12:A:ILE:HA   | 12       | 0.12          |
| (1,133) | 1:8:A:LEU:HB2 | 1:12:A:ILE:HG13 | 7        | 0.12          |
| (1,133) | 1:8:A:LEU:HB2 | 1:12:A:ILE:HG13 | 12       | 0.12          |
| (1,133) | 1:8:A:LEU:HB2 | 1:12:A:ILE:HG13 | 20       | 0.12          |
| (1,131) | 1:8:A:LEU:HA  | 1:12:A:ILE:HG12 | 6        | 0.12          |
| (1,131) | 1:8:A:LEU:HA  | 1:12:A:ILE:HG12 | 20       | 0.12          |
| (1,128) | 1:8:A:LEU:HA  | 1:76:A:LEU:HB3  | 5        | 0.12          |
| (1,128) | 1:8:A:LEU:HA  | 1:76:A:LEU:HB3  | 19       | 0.12          |
| (1,127) | 1:8:A:LEU:HA  | 1:12:A:ILE:HB   | 4        | 0.12          |
| (1,125) | 1:8:A:LEU:HB3 | 1:77:A:VAL:HA   | 3        | 0.12          |
| (1,125) | 1:8:A:LEU:HB3 | 1:77:A:VAL:HA   | 6        | 0.12          |
| (1,125) | 1:8:A:LEU:HB3 | 1:77:A:VAL:HA   | 10       | 0.12          |
| (1,125) | 1:8:A:LEU:HB3 | 1:77:A:VAL:HA   | 11       | 0.12          |
| (1,125) | 1:8:A:LEU:HB3 | 1:77:A:VAL:HA   | 14       | 0.12          |
| (1,125) | 1:8:A:LEU:HB3 | 1:77:A:VAL:HA   | 15       | 0.12          |
| (1,125) | 1:8:A:LEU:HB3 | 1:77:A:VAL:HA   | 20       | 0.12          |
| (1,113) | 1:7:A:GLU:HA  | 1:11:A:MET:HB3  | 6        | 0.12          |
| (1,113) | 1:7:A:GLU:HA  | 1:11:A:MET:HB3  | 15       | 0.12          |
| (1,112) | 1:7:A:GLU:HB3 | 1:10:A:GLN:HB2  | 1        | 0.12          |
| (1,112) | 1:7:A:GLU:HB3 | 1:10:A:GLN:HB2  | 7        | 0.12          |
| (1,112) | 1:7:A:GLU:HB3 | 1:10:A:GLN:HB2  | 8        | 0.12          |
| (1,112) | 1:7:A:GLU:HB3 | 1:10:A:GLN:HB2  | 12       | 0.12          |
| (1,111) | 1:7:A:GLU:H   | 1:10:A:GLN:HB2  | 4        | 0.12          |
| (1,111) | 1:7:A:GLU:H   | 1:10:A:GLN:HB2  | 8        | 0.12          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,111) | 1:7:A:GLU:H   | 1:10:A:GLN:HB2  | 18       | 0.12          |
| (1,111) | 1:7:A:GLU:H   | 1:10:A:GLN:HB2  | 19       | 0.12          |
| (1,95)  | 1:6:A:ASP:HB2 | 1:8:A:LEU:H     | 20       | 0.12          |
| (1,66)  | 1:5:A:ALA:HA  | 1:73:A:ILE:HG13 | 20       | 0.12          |
| (1,27)  | 1:4:A:LEU:HB2 | 1:84:A:GLN:HG3  | 7        | 0.12          |
| (1,27)  | 1:4:A:LEU:HB2 | 1:84:A:GLN:HG3  | 8        | 0.12          |
| (1,27)  | 1:4:A:LEU:HB2 | 1:84:A:GLN:HG3  | 15       | 0.12          |
| (1,26)  | 1:4:A:LEU:HB3 | 1:81:A:GLU:HA   | 1        | 0.12          |
| (1,26)  | 1:4:A:LEU:HB3 | 1:81:A:GLU:HA   | 4        | 0.12          |
| (1,26)  | 1:4:A:LEU:HB3 | 1:81:A:GLU:HA   | 6        | 0.12          |
| (1,26)  | 1:4:A:LEU:HB3 | 1:81:A:GLU:HA   | 7        | 0.12          |
| (1,26)  | 1:4:A:LEU:HB3 | 1:81:A:GLU:HA   | 13       | 0.12          |
| (1,23)  | 1:4:A:LEU:HA  | 1:8:A:LEU:HB2   | 20       | 0.12          |
| (1,22)  | 1:4:A:LEU:HB2 | 1:77:A:VAL:HA   | 1        | 0.12          |
| (1,22)  | 1:4:A:LEU:HB2 | 1:77:A:VAL:HA   | 2        | 0.12          |
| (1,22)  | 1:4:A:LEU:HB2 | 1:77:A:VAL:HA   | 16       | 0.12          |
| (1,19)  | 1:4:A:LEU:HG  | 1:81:A:GLU:HA   | 6        | 0.12          |
| (1,19)  | 1:4:A:LEU:HG  | 1:81:A:GLU:HA   | 11       | 0.12          |
| (1,18)  | 1:4:A:LEU:HA  | 1:8:A:LEU:HA    | 4        | 0.12          |
| (1,18)  | 1:4:A:LEU:HA  | 1:8:A:LEU:HA    | 6        | 0.12          |
| (1,18)  | 1:4:A:LEU:HA  | 1:8:A:LEU:HA    | 16       | 0.12          |
| (1,18)  | 1:4:A:LEU:HA  | 1:8:A:LEU:HA    | 19       | 0.12          |
| (1,16)  | 1:4:A:LEU:HB2 | 1:77:A:VAL:HB   | 3        | 0.12          |
| (1,16)  | 1:4:A:LEU:HB2 | 1:77:A:VAL:HB   | 13       | 0.12          |
| (1,16)  | 1:4:A:LEU:HB2 | 1:77:A:VAL:HB   | 17       | 0.12          |
| (1,15)  | 1:4:A:LEU:HG  | 1:7:A:GLU:HB2   | 4        | 0.12          |
| (1,15)  | 1:4:A:LEU:HG  | 1:7:A:GLU:HB2   | 17       | 0.12          |
| (1,15)  | 1:4:A:LEU:HG  | 1:7:A:GLU:HB2   | 19       | 0.12          |
| (1,14)  | 1:4:A:LEU:HB2 | 1:8:A:LEU:HB2   | 7        | 0.12          |
| (1,14)  | 1:4:A:LEU:HB2 | 1:8:A:LEU:HB2   | 9        | 0.12          |
| (1,14)  | 1:4:A:LEU:HB2 | 1:8:A:LEU:HB2   | 10       | 0.12          |
| (1,13)  | 1:4:A:LEU:HG  | 1:8:A:LEU:HA    | 4        | 0.12          |
| (1,13)  | 1:4:A:LEU:HG  | 1:8:A:LEU:HA    | 17       | 0.12          |
| (1,13)  | 1:4:A:LEU:HG  | 1:8:A:LEU:HA    | 19       | 0.12          |
| (1,12)  | 1:4:A:LEU:HA  | 1:7:A:GLU:HA    | 1        | 0.12          |
| (1,12)  | 1:4:A:LEU:HA  | 1:7:A:GLU:HA    | 5        | 0.12          |
| (1,12)  | 1:4:A:LEU:HA  | 1:7:A:GLU:HA    | 6        | 0.12          |
| (1,12)  | 1:4:A:LEU:HA  | 1:7:A:GLU:HA    | 8        | 0.12          |
| (1,12)  | 1:4:A:LEU:HA  | 1:7:A:GLU:HA    | 18       | 0.12          |
| (1,7)   | 1:3:A:ASN:H   | 1:84:A:GLN:HE22 | 1        | 0.12          |
| (1,7)   | 1:3:A:ASN:H   | 1:84:A:GLN:HE22 | 3        | 0.12          |
| (1,7)   | 1:3:A:ASN:H   | 1:84:A:GLN:HE22 | 7        | 0.12          |

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| Key    | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|--------|--------------|-----------------|----------|---------------|
| (1,7)  | 1:3:A:ASN:H  | 1:84:A:GLN:HE22 | 11       | 0.12          |
| (1,7)  | 1:3:A:ASN:H  | 1:84:A:GLN:HE22 | 15       | 0.12          |
| (1,2)  | 1:2:A:SER:H  | 1:4:A:LEU:HB3   | 6        | 0.12          |
| (2,71) | 1:78:A:ALA:O | 1:82:A:ALA:H    | 2        | 0.11          |
| (2,71) | 1:78:A:ALA:O | 1:82:A:ALA:H    | 4        | 0.11          |
| (2,71) | 1:78:A:ALA:O | 1:82:A:ALA:H    | 6        | 0.11          |
| (2,71) | 1:78:A:ALA:O | 1:82:A:ALA:H    | 8        | 0.11          |
| (2,71) | 1:78:A:ALA:O | 1:82:A:ALA:H    | 10       | 0.11          |
| (2,71) | 1:78:A:ALA:O | 1:82:A:ALA:H    | 11       | 0.11          |
| (2,71) | 1:78:A:ALA:O | 1:82:A:ALA:H    | 13       | 0.11          |
| (2,71) | 1:78:A:ALA:O | 1:82:A:ALA:H    | 18       | 0.11          |
| (2,71) | 1:78:A:ALA:O | 1:82:A:ALA:H    | 19       | 0.11          |
| (2,69) | 1:77:A:VAL:O | 1:81:A:GLU:N    | 20       | 0.11          |
| (2,51) | 1:63:A:SER:O | 1:67:A:LYS:H    | 11       | 0.11          |
| (2,51) | 1:63:A:SER:O | 1:67:A:LYS:H    | 13       | 0.11          |
| (2,51) | 1:63:A:SER:O | 1:67:A:LYS:H    | 16       | 0.11          |
| (2,49) | 1:52:A:LYS:O | 1:56:A:ASN:N    | 4        | 0.11          |
| (2,49) | 1:52:A:LYS:O | 1:56:A:ASN:N    | 18       | 0.11          |
| (2,33) | 1:44:A:ALA:O | 1:48:A:GLY:N    | 10       | 0.11          |
| (2,15) | 1:11:A:MET:O | 1:15:A:VAL:N    | 4        | 0.11          |
| (2,15) | 1:11:A:MET:O | 1:15:A:VAL:N    | 7        | 0.11          |
| (2,14) | 1:10:A:GLN:O | 1:14:A:ASP:N    | 6        | 0.11          |
| (2,14) | 1:10:A:GLN:O | 1:14:A:ASP:N    | 9        | 0.11          |
| (2,14) | 1:10:A:GLN:O | 1:14:A:ASP:N    | 12       | 0.11          |
| (2,14) | 1:10:A:GLN:O | 1:14:A:ASP:N    | 17       | 0.11          |
| (2,14) | 1:10:A:GLN:O | 1:14:A:ASP:N    | 18       | 0.11          |
| (2,9)  | 1:8:A:LEU:O  | 1:12:A:ILE:N    | 4        | 0.11          |
| (2,9)  | 1:8:A:LEU:O  | 1:12:A:ILE:N    | 19       | 0.11          |
| (2,8)  | 1:7:A:GLU:O  | 1:11:A:MET:N    | 4        | 0.11          |
| (2,8)  | 1:7:A:GLU:O  | 1:11:A:MET:N    | 7        | 0.11          |
| (2,8)  | 1:7:A:GLU:O  | 1:11:A:MET:N    | 10       | 0.11          |
| (2,8)  | 1:7:A:GLU:O  | 1:11:A:MET:N    | 12       | 0.11          |
| (2,8)  | 1:7:A:GLU:O  | 1:11:A:MET:N    | 17       | 0.11          |
| (2,8)  | 1:7:A:GLU:O  | 1:11:A:MET:N    | 19       | 0.11          |
| (2,8)  | 1:7:A:GLU:O  | 1:11:A:MET:N    | 20       | 0.11          |
| (2,1)  | 1:4:A:LEU:O  | 1:8:A:LEU:N     | 1        | 0.11          |
| (2,1)  | 1:4:A:LEU:O  | 1:8:A:LEU:N     | 3        | 0.11          |
| (2,1)  | 1:4:A:LEU:O  | 1:8:A:LEU:N     | 5        | 0.11          |
| (2,1)  | 1:4:A:LEU:O  | 1:8:A:LEU:N     | 6        | 0.11          |
| (2,1)  | 1:4:A:LEU:O  | 1:8:A:LEU:N     | 7        | 0.11          |
| (2,1)  | 1:4:A:LEU:O  | 1:8:A:LEU:N     | 9        | 0.11          |
| (2,1)  | 1:4:A:LEU:O  | 1:8:A:LEU:N     | 10       | 0.11          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (2,1)    | 1:4:A:LEU:O    | 1:8:A:LEU:N    | 11       | 0.11          |
| (2,1)    | 1:4:A:LEU:O    | 1:8:A:LEU:N    | 12       | 0.11          |
| (2,1)    | 1:4:A:LEU:O    | 1:8:A:LEU:N    | 13       | 0.11          |
| (2,1)    | 1:4:A:LEU:O    | 1:8:A:LEU:N    | 14       | 0.11          |
| (2,1)    | 1:4:A:LEU:O    | 1:8:A:LEU:N    | 16       | 0.11          |
| (2,1)    | 1:4:A:LEU:O    | 1:8:A:LEU:N    | 17       | 0.11          |
| (1,1227) | 1:84:A:GLN:H   | 1:85:A:LYS:HB2 | 8        | 0.11          |
| (1,1227) | 1:84:A:GLN:H   | 1:85:A:LYS:HB2 | 10       | 0.11          |
| (1,1217) | 1:83:A:GLN:H   | 1:85:A:LYS:H   | 17       | 0.11          |
| (1,1213) | 1:82:A:ALA:HA  | 1:84:A:GLN:H   | 3        | 0.11          |
| (1,1213) | 1:82:A:ALA:HA  | 1:84:A:GLN:H   | 10       | 0.11          |
| (1,1213) | 1:82:A:ALA:HA  | 1:84:A:GLN:H   | 14       | 0.11          |
| (1,1213) | 1:82:A:ALA:HA  | 1:84:A:GLN:H   | 16       | 0.11          |
| (1,1175) | 1:80:A:VAL:HA  | 1:84:A:GLN:HG2 | 6        | 0.11          |
| (1,1175) | 1:80:A:VAL:HA  | 1:84:A:GLN:HG2 | 19       | 0.11          |
| (1,1169) | 1:80:A:VAL:HB  | 1:84:A:GLN:HG2 | 12       | 0.11          |
| (1,1168) | 1:80:A:VAL:HA  | 1:83:A:GLN:HA  | 5        | 0.11          |
| (1,1168) | 1:80:A:VAL:HA  | 1:83:A:GLN:HA  | 18       | 0.11          |
| (1,1168) | 1:80:A:VAL:HA  | 1:83:A:GLN:HA  | 20       | 0.11          |
| (1,1158) | 1:79:A:LEU:HB3 | 1:82:A:ALA:H   | 3        | 0.11          |
| (1,1158) | 1:79:A:LEU:HB3 | 1:82:A:ALA:H   | 9        | 0.11          |
| (1,1158) | 1:79:A:LEU:HB3 | 1:82:A:ALA:H   | 10       | 0.11          |
| (1,1158) | 1:79:A:LEU:HB3 | 1:82:A:ALA:H   | 19       | 0.11          |
| (1,1157) | 1:79:A:LEU:H   | 1:81:A:GLU:H   | 1        | 0.11          |
| (1,1157) | 1:79:A:LEU:H   | 1:81:A:GLU:H   | 4        | 0.11          |
| (1,1157) | 1:79:A:LEU:H   | 1:81:A:GLU:H   | 9        | 0.11          |
| (1,1157) | 1:79:A:LEU:H   | 1:81:A:GLU:H   | 14       | 0.11          |
| (1,1157) | 1:79:A:LEU:H   | 1:81:A:GLU:H   | 17       | 0.11          |
| (1,1156) | 1:79:A:LEU:HB2 | 1:82:A:ALA:H   | 1        | 0.11          |
| (1,1156) | 1:79:A:LEU:HB2 | 1:82:A:ALA:H   | 6        | 0.11          |
| (1,1156) | 1:79:A:LEU:HB2 | 1:82:A:ALA:H   | 13       | 0.11          |
| (1,1156) | 1:79:A:LEU:HB2 | 1:82:A:ALA:H   | 18       | 0.11          |
| (1,1156) | 1:79:A:LEU:HB2 | 1:82:A:ALA:H   | 19       | 0.11          |
| (1,1149) | 1:78:A:ALA:H   | 1:82:A:ALA:H   | 2        | 0.11          |
| (1,1149) | 1:78:A:ALA:H   | 1:82:A:ALA:H   | 5        | 0.11          |
| (1,1149) | 1:78:A:ALA:H   | 1:82:A:ALA:H   | 8        | 0.11          |
| (1,1149) | 1:78:A:ALA:H   | 1:82:A:ALA:H   | 10       | 0.11          |
| (1,1149) | 1:78:A:ALA:H   | 1:82:A:ALA:H   | 15       | 0.11          |
| (1,1149) | 1:78:A:ALA:H   | 1:82:A:ALA:H   | 18       | 0.11          |
| (1,1145) | 1:78:A:ALA:H   | 1:80:A:VAL:H   | 1        | 0.11          |
| (1,1145) | 1:78:A:ALA:H   | 1:80:A:VAL:H   | 2        | 0.11          |
| (1,1145) | 1:78:A:ALA:H   | 1:80:A:VAL:H   | 6        | 0.11          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1145) | 1:78:A:ALA:H    | 1:80:A:VAL:H   | 10       | 0.11          |
| (1,1145) | 1:78:A:ALA:H    | 1:80:A:VAL:H   | 17       | 0.11          |
| (1,1145) | 1:78:A:ALA:H    | 1:80:A:VAL:H   | 18       | 0.11          |
| (1,1126) | 1:77:A:VAL:HA   | 1:81:A:GLU:HA  | 12       | 0.11          |
| (1,1121) | 1:77:A:VAL:HA   | 1:80:A:VAL:HA  | 7        | 0.11          |
| (1,1118) | 1:77:A:VAL:HB   | 1:81:A:GLU:H   | 5        | 0.11          |
| (1,1118) | 1:77:A:VAL:HB   | 1:81:A:GLU:H   | 7        | 0.11          |
| (1,1118) | 1:77:A:VAL:HB   | 1:81:A:GLU:H   | 8        | 0.11          |
| (1,1113) | 1:77:A:VAL:HB   | 1:79:A:LEU:H   | 1        | 0.11          |
| (1,1113) | 1:77:A:VAL:HB   | 1:79:A:LEU:H   | 9        | 0.11          |
| (1,1113) | 1:77:A:VAL:HB   | 1:79:A:LEU:H   | 10       | 0.11          |
| (1,1113) | 1:77:A:VAL:HB   | 1:79:A:LEU:H   | 11       | 0.11          |
| (1,1113) | 1:77:A:VAL:HB   | 1:79:A:LEU:H   | 14       | 0.11          |
| (1,1113) | 1:77:A:VAL:HB   | 1:79:A:LEU:H   | 17       | 0.11          |
| (1,1113) | 1:77:A:VAL:HB   | 1:79:A:LEU:H   | 19       | 0.11          |
| (1,1091) | 1:76:A:LEU:HG   | 1:79:A:LEU:HB2 | 6        | 0.11          |
| (1,1091) | 1:76:A:LEU:HG   | 1:79:A:LEU:HB2 | 9        | 0.11          |
| (1,1091) | 1:76:A:LEU:HG   | 1:79:A:LEU:HB2 | 17       | 0.11          |
| (1,1080) | 1:75:A:SER:HB3  | 1:79:A:LEU:HG  | 5        | 0.11          |
| (1,1080) | 1:75:A:SER:HB3  | 1:79:A:LEU:HG  | 7        | 0.11          |
| (1,1080) | 1:75:A:SER:HB3  | 1:79:A:LEU:HG  | 8        | 0.11          |
| (1,1080) | 1:75:A:SER:HB3  | 1:79:A:LEU:HG  | 10       | 0.11          |
| (1,1078) | 1:75:A:SER:HB2  | 1:79:A:LEU:H   | 2        | 0.11          |
| (1,1078) | 1:75:A:SER:HB2  | 1:79:A:LEU:H   | 10       | 0.11          |
| (1,1078) | 1:75:A:SER:HB2  | 1:79:A:LEU:H   | 13       | 0.11          |
| (1,1078) | 1:75:A:SER:HB2  | 1:79:A:LEU:H   | 15       | 0.11          |
| (1,1078) | 1:75:A:SER:HB2  | 1:79:A:LEU:H   | 19       | 0.11          |
| (1,1064) | 1:74:A:GLN:H    | 1:77:A:VAL:HB  | 2        | 0.11          |
| (1,1064) | 1:74:A:GLN:H    | 1:77:A:VAL:HB  | 4        | 0.11          |
| (1,1064) | 1:74:A:GLN:H    | 1:77:A:VAL:HB  | 10       | 0.11          |
| (1,1064) | 1:74:A:GLN:H    | 1:77:A:VAL:HB  | 12       | 0.11          |
| (1,1064) | 1:74:A:GLN:H    | 1:77:A:VAL:HB  | 20       | 0.11          |
| (1,1039) | 1:73:A:ILE:HB   | 1:76:A:LEU:HG  | 11       | 0.11          |
| (1,1039) | 1:73:A:ILE:HB   | 1:76:A:LEU:HG  | 15       | 0.11          |
| (1,1039) | 1:73:A:ILE:HB   | 1:76:A:LEU:HG  | 17       | 0.11          |
| (1,1035) | 1:73:A:ILE:HG12 | 1:76:A:LEU:HB2 | 7        | 0.11          |
| (1,1035) | 1:73:A:ILE:HG12 | 1:76:A:LEU:HB2 | 12       | 0.11          |
| (1,1035) | 1:73:A:ILE:HG12 | 1:76:A:LEU:HB2 | 17       | 0.11          |
| (1,1035) | 1:73:A:ILE:HG12 | 1:76:A:LEU:HB2 | 20       | 0.11          |
| (1,1034) | 1:73:A:ILE:HB   | 1:77:A:VAL:HB  | 3        | 0.11          |
| (1,1034) | 1:73:A:ILE:HB   | 1:77:A:VAL:HB  | 9        | 0.11          |
| (1,1034) | 1:73:A:ILE:HB   | 1:77:A:VAL:HB  | 13       | 0.11          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1034) | 1:73:A:ILE:HB  | 1:77:A:VAL:HB  | 14       | 0.11          |
| (1,1034) | 1:73:A:ILE:HB  | 1:77:A:VAL:HB  | 18       | 0.11          |
| (1,1034) | 1:73:A:ILE:HB  | 1:77:A:VAL:HB  | 20       | 0.11          |
| (1,1033) | 1:73:A:ILE:HA  | 1:77:A:VAL:HA  | 2        | 0.11          |
| (1,1033) | 1:73:A:ILE:HA  | 1:77:A:VAL:HA  | 5        | 0.11          |
| (1,1033) | 1:73:A:ILE:HA  | 1:77:A:VAL:HA  | 6        | 0.11          |
| (1,1033) | 1:73:A:ILE:HA  | 1:77:A:VAL:HA  | 14       | 0.11          |
| (1,1033) | 1:73:A:ILE:HA  | 1:77:A:VAL:HA  | 18       | 0.11          |
| (1,1032) | 1:73:A:ILE:H   | 1:76:A:LEU:HG  | 1        | 0.11          |
| (1,1032) | 1:73:A:ILE:H   | 1:76:A:LEU:HG  | 4        | 0.11          |
| (1,1032) | 1:73:A:ILE:H   | 1:76:A:LEU:HG  | 5        | 0.11          |
| (1,1032) | 1:73:A:ILE:H   | 1:76:A:LEU:HG  | 9        | 0.11          |
| (1,1032) | 1:73:A:ILE:H   | 1:76:A:LEU:HG  | 12       | 0.11          |
| (1,1032) | 1:73:A:ILE:H   | 1:76:A:LEU:HG  | 13       | 0.11          |
| (1,1032) | 1:73:A:ILE:H   | 1:76:A:LEU:HG  | 14       | 0.11          |
| (1,1032) | 1:73:A:ILE:H   | 1:76:A:LEU:HG  | 15       | 0.11          |
| (1,1032) | 1:73:A:ILE:H   | 1:76:A:LEU:HG  | 16       | 0.11          |
| (1,1032) | 1:73:A:ILE:H   | 1:76:A:LEU:HG  | 19       | 0.11          |
| (1,988)  | 1:70:A:PHE:HB2 | 1:76:A:LEU:HG  | 9        | 0.11          |
| (1,988)  | 1:70:A:PHE:HB2 | 1:76:A:LEU:HG  | 17       | 0.11          |
| (1,986)  | 1:70:A:PHE:HB3 | 1:75:A:SER:HB2 | 1        | 0.11          |
| (1,985)  | 1:70:A:PHE:HB2 | 1:75:A:SER:HB2 | 3        | 0.11          |
| (1,985)  | 1:70:A:PHE:HB2 | 1:75:A:SER:HB2 | 4        | 0.11          |
| (1,985)  | 1:70:A:PHE:HB2 | 1:75:A:SER:HB2 | 5        | 0.11          |
| (1,985)  | 1:70:A:PHE:HB2 | 1:75:A:SER:HB2 | 7        | 0.11          |
| (1,985)  | 1:70:A:PHE:HB2 | 1:75:A:SER:HB2 | 8        | 0.11          |
| (1,985)  | 1:70:A:PHE:HB2 | 1:75:A:SER:HB2 | 15       | 0.11          |
| (1,985)  | 1:70:A:PHE:HB2 | 1:75:A:SER:HB2 | 19       | 0.11          |
| (1,985)  | 1:70:A:PHE:HB2 | 1:75:A:SER:HB2 | 20       | 0.11          |
| (1,963)  | 1:69:A:HIS:HA  | 1:76:A:LEU:HA  | 7        | 0.11          |
| (1,963)  | 1:69:A:HIS:HA  | 1:76:A:LEU:HA  | 15       | 0.11          |
| (1,963)  | 1:69:A:HIS:HA  | 1:76:A:LEU:HA  | 19       | 0.11          |
| (1,962)  | 1:69:A:HIS:HB2 | 1:76:A:LEU:HG  | 6        | 0.11          |
| (1,962)  | 1:69:A:HIS:HB2 | 1:76:A:LEU:HG  | 13       | 0.11          |
| (1,961)  | 1:69:A:HIS:H   | 1:75:A:SER:HB2 | 1        | 0.11          |
| (1,961)  | 1:69:A:HIS:H   | 1:75:A:SER:HB2 | 2        | 0.11          |
| (1,961)  | 1:69:A:HIS:H   | 1:75:A:SER:HB2 | 4        | 0.11          |
| (1,961)  | 1:69:A:HIS:H   | 1:75:A:SER:HB2 | 8        | 0.11          |
| (1,961)  | 1:69:A:HIS:H   | 1:75:A:SER:HB2 | 10       | 0.11          |
| (1,961)  | 1:69:A:HIS:H   | 1:75:A:SER:HB2 | 14       | 0.11          |
| (1,961)  | 1:69:A:HIS:H   | 1:75:A:SER:HB2 | 16       | 0.11          |
| (1,961)  | 1:69:A:HIS:H   | 1:75:A:SER:HB2 | 18       | 0.11          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,959) | 1:69:A:HIS:HB2 | 1:79:A:LEU:H   | 17       | 0.11          |
| (1,951) | 1:67:A:LYS:HA  | 1:71:A:LYS:H   | 15       | 0.11          |
| (1,951) | 1:67:A:LYS:HA  | 1:71:A:LYS:H   | 16       | 0.11          |
| (1,943) | 1:66:A:THR:HB  | 1:69:A:HIS:H   | 2        | 0.11          |
| (1,943) | 1:66:A:THR:HB  | 1:69:A:HIS:H   | 6        | 0.11          |
| (1,943) | 1:66:A:THR:HB  | 1:69:A:HIS:H   | 8        | 0.11          |
| (1,943) | 1:66:A:THR:HB  | 1:69:A:HIS:H   | 10       | 0.11          |
| (1,943) | 1:66:A:THR:HB  | 1:69:A:HIS:H   | 11       | 0.11          |
| (1,942) | 1:66:A:THR:HB  | 1:68:A:GLN:H   | 2        | 0.11          |
| (1,942) | 1:66:A:THR:HB  | 1:68:A:GLN:H   | 6        | 0.11          |
| (1,942) | 1:66:A:THR:HB  | 1:68:A:GLN:H   | 7        | 0.11          |
| (1,942) | 1:66:A:THR:HB  | 1:68:A:GLN:H   | 8        | 0.11          |
| (1,942) | 1:66:A:THR:HB  | 1:68:A:GLN:H   | 11       | 0.11          |
| (1,942) | 1:66:A:THR:HB  | 1:68:A:GLN:H   | 13       | 0.11          |
| (1,942) | 1:66:A:THR:HB  | 1:68:A:GLN:H   | 14       | 0.11          |
| (1,942) | 1:66:A:THR:HB  | 1:68:A:GLN:H   | 16       | 0.11          |
| (1,942) | 1:66:A:THR:HB  | 1:68:A:GLN:H   | 17       | 0.11          |
| (1,942) | 1:66:A:THR:HB  | 1:68:A:GLN:H   | 19       | 0.11          |
| (1,941) | 1:66:A:THR:H   | 1:68:A:GLN:HG2 | 5        | 0.11          |
| (1,941) | 1:66:A:THR:H   | 1:68:A:GLN:HG2 | 11       | 0.11          |
| (1,941) | 1:66:A:THR:H   | 1:68:A:GLN:HG2 | 12       | 0.11          |
| (1,940) | 1:66:A:THR:H   | 1:70:A:PHE:H   | 6        | 0.11          |
| (1,940) | 1:66:A:THR:H   | 1:70:A:PHE:H   | 8        | 0.11          |
| (1,940) | 1:66:A:THR:H   | 1:70:A:PHE:H   | 15       | 0.11          |
| (1,940) | 1:66:A:THR:H   | 1:70:A:PHE:H   | 16       | 0.11          |
| (1,940) | 1:66:A:THR:H   | 1:70:A:PHE:H   | 18       | 0.11          |
| (1,940) | 1:66:A:THR:H   | 1:70:A:PHE:H   | 19       | 0.11          |
| (1,939) | 1:66:A:THR:H   | 1:68:A:GLN:H   | 1        | 0.11          |
| (1,939) | 1:66:A:THR:H   | 1:68:A:GLN:H   | 2        | 0.11          |
| (1,939) | 1:66:A:THR:H   | 1:68:A:GLN:H   | 3        | 0.11          |
| (1,939) | 1:66:A:THR:H   | 1:68:A:GLN:H   | 4        | 0.11          |
| (1,939) | 1:66:A:THR:H   | 1:68:A:GLN:H   | 5        | 0.11          |
| (1,939) | 1:66:A:THR:H   | 1:68:A:GLN:H   | 6        | 0.11          |
| (1,939) | 1:66:A:THR:H   | 1:68:A:GLN:H   | 7        | 0.11          |
| (1,939) | 1:66:A:THR:H   | 1:68:A:GLN:H   | 9        | 0.11          |
| (1,939) | 1:66:A:THR:H   | 1:68:A:GLN:H   | 10       | 0.11          |
| (1,939) | 1:66:A:THR:H   | 1:68:A:GLN:H   | 12       | 0.11          |
| (1,939) | 1:66:A:THR:H   | 1:68:A:GLN:H   | 14       | 0.11          |
| (1,939) | 1:66:A:THR:H   | 1:68:A:GLN:H   | 15       | 0.11          |
| (1,939) | 1:66:A:THR:H   | 1:68:A:GLN:H   | 17       | 0.11          |
| (1,939) | 1:66:A:THR:H   | 1:68:A:GLN:H   | 19       | 0.11          |
| (1,939) | 1:66:A:THR:H   | 1:68:A:GLN:H   | 20       | 0.11          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,938) | 1:66:A:THR:H  | 1:69:A:HIS:H   | 6        | 0.11          |
| (1,938) | 1:66:A:THR:H  | 1:69:A:HIS:H   | 8        | 0.11          |
| (1,938) | 1:66:A:THR:H  | 1:69:A:HIS:H   | 12       | 0.11          |
| (1,938) | 1:66:A:THR:H  | 1:69:A:HIS:H   | 14       | 0.11          |
| (1,938) | 1:66:A:THR:H  | 1:69:A:HIS:H   | 18       | 0.11          |
| (1,937) | 1:66:A:THR:H  | 1:68:A:GLN:HG3 | 1        | 0.11          |
| (1,937) | 1:66:A:THR:H  | 1:68:A:GLN:HG3 | 3        | 0.11          |
| (1,937) | 1:66:A:THR:H  | 1:68:A:GLN:HG3 | 4        | 0.11          |
| (1,937) | 1:66:A:THR:H  | 1:68:A:GLN:HG3 | 5        | 0.11          |
| (1,937) | 1:66:A:THR:H  | 1:68:A:GLN:HG3 | 8        | 0.11          |
| (1,937) | 1:66:A:THR:H  | 1:68:A:GLN:HG3 | 9        | 0.11          |
| (1,937) | 1:66:A:THR:H  | 1:68:A:GLN:HG3 | 11       | 0.11          |
| (1,937) | 1:66:A:THR:H  | 1:68:A:GLN:HG3 | 12       | 0.11          |
| (1,937) | 1:66:A:THR:H  | 1:68:A:GLN:HG3 | 14       | 0.11          |
| (1,937) | 1:66:A:THR:H  | 1:68:A:GLN:HG3 | 15       | 0.11          |
| (1,937) | 1:66:A:THR:H  | 1:68:A:GLN:HG3 | 16       | 0.11          |
| (1,937) | 1:66:A:THR:H  | 1:68:A:GLN:HG3 | 18       | 0.11          |
| (1,937) | 1:66:A:THR:H  | 1:68:A:GLN:HG3 | 19       | 0.11          |
| (1,937) | 1:66:A:THR:H  | 1:68:A:GLN:HG3 | 20       | 0.11          |
| (1,917) | 1:65:A:GLU:HA | 1:68:A:GLN:HA  | 6        | 0.11          |
| (1,917) | 1:65:A:GLU:HA | 1:68:A:GLN:HA  | 9        | 0.11          |
| (1,917) | 1:65:A:GLU:HA | 1:68:A:GLN:HA  | 10       | 0.11          |
| (1,917) | 1:65:A:GLU:HA | 1:68:A:GLN:HA  | 11       | 0.11          |
| (1,903) | 1:64:A:ASP:H  | 1:67:A:LYS:H   | 2        | 0.11          |
| (1,903) | 1:64:A:ASP:H  | 1:67:A:LYS:H   | 9        | 0.11          |
| (1,903) | 1:64:A:ASP:H  | 1:67:A:LYS:H   | 10       | 0.11          |
| (1,903) | 1:64:A:ASP:H  | 1:67:A:LYS:H   | 13       | 0.11          |
| (1,897) | 1:64:A:ASP:H  | 1:68:A:GLN:H   | 1        | 0.11          |
| (1,897) | 1:64:A:ASP:H  | 1:68:A:GLN:H   | 2        | 0.11          |
| (1,897) | 1:64:A:ASP:H  | 1:68:A:GLN:H   | 4        | 0.11          |
| (1,897) | 1:64:A:ASP:H  | 1:68:A:GLN:H   | 7        | 0.11          |
| (1,897) | 1:64:A:ASP:H  | 1:68:A:GLN:H   | 10       | 0.11          |
| (1,897) | 1:64:A:ASP:H  | 1:68:A:GLN:H   | 12       | 0.11          |
| (1,897) | 1:64:A:ASP:H  | 1:68:A:GLN:H   | 14       | 0.11          |
| (1,897) | 1:64:A:ASP:H  | 1:68:A:GLN:H   | 16       | 0.11          |
| (1,897) | 1:64:A:ASP:H  | 1:68:A:GLN:H   | 18       | 0.11          |
| (1,897) | 1:64:A:ASP:H  | 1:68:A:GLN:H   | 19       | 0.11          |
| (1,897) | 1:64:A:ASP:H  | 1:68:A:GLN:H   | 20       | 0.11          |
| (1,892) | 1:63:A:SER:HA | 1:67:A:LYS:HG2 | 14       | 0.11          |
| (1,892) | 1:63:A:SER:HA | 1:67:A:LYS:HG2 | 16       | 0.11          |
| (1,891) | 1:63:A:SER:H  | 1:65:A:GLU:H   | 2        | 0.11          |
| (1,886) | 1:62:A:GLU:HA | 1:67:A:LYS:HG2 | 9        | 0.11          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,886) | 1:62:A:GLU:HA  | 1:67:A:LYS:HG2 | 18       | 0.11          |
| (1,877) | 1:61:A:ALA:HA  | 1:66:A:THR:H   | 16       | 0.11          |
| (1,877) | 1:61:A:ALA:HA  | 1:66:A:THR:H   | 18       | 0.11          |
| (1,876) | 1:60:A:ASN:HB3 | 1:66:A:THR:H   | 10       | 0.11          |
| (1,858) | 1:60:A:ASN:HA  | 1:66:A:THR:H   | 15       | 0.11          |
| (1,857) | 1:60:A:ASN:HB2 | 1:66:A:THR:HA  | 4        | 0.11          |
| (1,857) | 1:60:A:ASN:HB2 | 1:66:A:THR:HA  | 8        | 0.11          |
| (1,857) | 1:60:A:ASN:HB2 | 1:66:A:THR:HA  | 15       | 0.11          |
| (1,857) | 1:60:A:ASN:HB2 | 1:66:A:THR:HA  | 19       | 0.11          |
| (1,839) | 1:57:A:ILE:H   | 1:83:A:GLN:HG3 | 4        | 0.11          |
| (1,833) | 1:57:A:ILE:HA  | 1:59:A:LEU:H   | 5        | 0.11          |
| (1,833) | 1:57:A:ILE:HA  | 1:59:A:LEU:H   | 13       | 0.11          |
| (1,833) | 1:57:A:ILE:HA  | 1:59:A:LEU:H   | 18       | 0.11          |
| (1,829) | 1:57:A:ILE:HA  | 1:80:A:VAL:HA  | 5        | 0.11          |
| (1,829) | 1:57:A:ILE:HA  | 1:80:A:VAL:HA  | 7        | 0.11          |
| (1,800) | 1:55:A:TYR:HB3 | 1:80:A:VAL:HA  | 17       | 0.11          |
| (1,796) | 1:55:A:TYR:HB2 | 1:83:A:GLN:HB3 | 9        | 0.11          |
| (1,796) | 1:55:A:TYR:HB2 | 1:83:A:GLN:HB3 | 15       | 0.11          |
| (1,796) | 1:55:A:TYR:HB2 | 1:83:A:GLN:HB3 | 20       | 0.11          |
| (1,795) | 1:55:A:TYR:HB3 | 1:57:A:ILE:HA  | 6        | 0.11          |
| (1,795) | 1:55:A:TYR:HB3 | 1:57:A:ILE:HA  | 12       | 0.11          |
| (1,795) | 1:55:A:TYR:HB3 | 1:57:A:ILE:HA  | 15       | 0.11          |
| (1,795) | 1:55:A:TYR:HB3 | 1:57:A:ILE:HA  | 18       | 0.11          |
| (1,795) | 1:55:A:TYR:HB3 | 1:57:A:ILE:HA  | 19       | 0.11          |
| (1,794) | 1:55:A:TYR:HB2 | 1:84:A:GLN:HG2 | 12       | 0.11          |
| (1,789) | 1:54:A:ARG:H   | 1:55:A:TYR:HA  | 2        | 0.11          |
| (1,789) | 1:54:A:ARG:H   | 1:55:A:TYR:HA  | 4        | 0.11          |
| (1,789) | 1:54:A:ARG:H   | 1:55:A:TYR:HA  | 11       | 0.11          |
| (1,789) | 1:54:A:ARG:H   | 1:55:A:TYR:HA  | 12       | 0.11          |
| (1,766) | 1:52:A:LYS:HB3 | 1:59:A:LEU:H   | 11       | 0.11          |
| (1,763) | 1:52:A:LYS:HA  | 1:59:A:LEU:H   | 2        | 0.11          |
| (1,763) | 1:52:A:LYS:HA  | 1:59:A:LEU:H   | 11       | 0.11          |
| (1,761) | 1:52:A:LYS:HA  | 1:56:A:ASN:HB3 | 15       | 0.11          |
| (1,760) | 1:52:A:LYS:HA  | 1:56:A:ASN:HB2 | 18       | 0.11          |
| (1,758) | 1:52:A:LYS:HG3 | 1:57:A:ILE:H   | 2        | 0.11          |
| (1,758) | 1:52:A:LYS:HG3 | 1:57:A:ILE:H   | 5        | 0.11          |
| (1,758) | 1:52:A:LYS:HG3 | 1:57:A:ILE:H   | 6        | 0.11          |
| (1,758) | 1:52:A:LYS:HG3 | 1:57:A:ILE:H   | 10       | 0.11          |
| (1,758) | 1:52:A:LYS:HG3 | 1:57:A:ILE:H   | 11       | 0.11          |
| (1,742) | 1:51:A:LEU:HB2 | 1:59:A:LEU:HB2 | 12       | 0.11          |
| (1,741) | 1:51:A:LEU:H   | 1:52:A:LYS:HA  | 16       | 0.11          |
| (1,741) | 1:51:A:LEU:H   | 1:52:A:LYS:HA  | 17       | 0.11          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,739) | 1:51:A:LEU:HB3 | 1:54:A:ARG:HB3 | 4        | 0.11          |
| (1,737) | 1:51:A:LEU:HA  | 1:57:A:ILE:H   | 8        | 0.11          |
| (1,736) | 1:51:A:LEU:HB3 | 1:59:A:LEU:HG  | 5        | 0.11          |
| (1,736) | 1:51:A:LEU:HB3 | 1:59:A:LEU:HG  | 13       | 0.11          |
| (1,724) | 1:50:A:ALA:H   | 1:52:A:LYS:HB3 | 2        | 0.11          |
| (1,724) | 1:50:A:ALA:H   | 1:52:A:LYS:HB3 | 5        | 0.11          |
| (1,724) | 1:50:A:ALA:H   | 1:52:A:LYS:HB3 | 6        | 0.11          |
| (1,724) | 1:50:A:ALA:H   | 1:52:A:LYS:HB3 | 8        | 0.11          |
| (1,724) | 1:50:A:ALA:H   | 1:52:A:LYS:HB3 | 10       | 0.11          |
| (1,724) | 1:50:A:ALA:H   | 1:52:A:LYS:HB3 | 12       | 0.11          |
| (1,723) | 1:50:A:ALA:H   | 1:51:A:LEU:HA  | 2        | 0.11          |
| (1,723) | 1:50:A:ALA:H   | 1:51:A:LEU:HA  | 3        | 0.11          |
| (1,723) | 1:50:A:ALA:H   | 1:51:A:LEU:HA  | 4        | 0.11          |
| (1,723) | 1:50:A:ALA:H   | 1:51:A:LEU:HA  | 5        | 0.11          |
| (1,723) | 1:50:A:ALA:H   | 1:51:A:LEU:HA  | 6        | 0.11          |
| (1,723) | 1:50:A:ALA:H   | 1:51:A:LEU:HA  | 7        | 0.11          |
| (1,723) | 1:50:A:ALA:H   | 1:51:A:LEU:HA  | 8        | 0.11          |
| (1,723) | 1:50:A:ALA:H   | 1:51:A:LEU:HA  | 11       | 0.11          |
| (1,723) | 1:50:A:ALA:H   | 1:51:A:LEU:HA  | 12       | 0.11          |
| (1,723) | 1:50:A:ALA:H   | 1:51:A:LEU:HA  | 14       | 0.11          |
| (1,723) | 1:50:A:ALA:H   | 1:51:A:LEU:HA  | 15       | 0.11          |
| (1,723) | 1:50:A:ALA:H   | 1:51:A:LEU:HA  | 18       | 0.11          |
| (1,723) | 1:50:A:ALA:H   | 1:51:A:LEU:HA  | 20       | 0.11          |
| (1,722) | 1:50:A:ALA:HA  | 1:52:A:LYS:HB3 | 4        | 0.11          |
| (1,722) | 1:50:A:ALA:HA  | 1:52:A:LYS:HB3 | 6        | 0.11          |
| (1,722) | 1:50:A:ALA:HA  | 1:52:A:LYS:HB3 | 11       | 0.11          |
| (1,708) | 1:49:A:LEU:HB2 | 1:52:A:LYS:H   | 1        | 0.11          |
| (1,708) | 1:49:A:LEU:HB2 | 1:52:A:LYS:H   | 6        | 0.11          |
| (1,708) | 1:49:A:LEU:HB2 | 1:52:A:LYS:H   | 7        | 0.11          |
| (1,707) | 1:49:A:LEU:HA  | 1:53:A:LYS:H   | 4        | 0.11          |
| (1,707) | 1:49:A:LEU:HA  | 1:53:A:LYS:H   | 6        | 0.11          |
| (1,707) | 1:49:A:LEU:HA  | 1:53:A:LYS:H   | 7        | 0.11          |
| (1,693) | 1:48:A:GLY:HA3 | 1:51:A:LEU:HG  | 1        | 0.11          |
| (1,693) | 1:48:A:GLY:HA3 | 1:51:A:LEU:HG  | 4        | 0.11          |
| (1,692) | 1:48:A:GLY:HA2 | 1:51:A:LEU:HA  | 6        | 0.11          |
| (1,692) | 1:48:A:GLY:HA2 | 1:51:A:LEU:HA  | 13       | 0.11          |
| (1,691) | 1:48:A:GLY:HA3 | 1:51:A:LEU:HB3 | 2        | 0.11          |
| (1,691) | 1:48:A:GLY:HA3 | 1:51:A:LEU:HB3 | 9        | 0.11          |
| (1,691) | 1:48:A:GLY:HA3 | 1:51:A:LEU:HB3 | 15       | 0.11          |
| (1,689) | 1:48:A:GLY:HA3 | 1:52:A:LYS:HB2 | 2        | 0.11          |
| (1,689) | 1:48:A:GLY:HA3 | 1:52:A:LYS:HB2 | 14       | 0.11          |
| (1,689) | 1:48:A:GLY:HA3 | 1:52:A:LYS:HB2 | 16       | 0.11          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,688) | 1:48:A:GLY:HA2 | 1:59:A:LEU:HB3 | 10       | 0.11          |
| (1,688) | 1:48:A:GLY:HA2 | 1:59:A:LEU:HB3 | 12       | 0.11          |
| (1,688) | 1:48:A:GLY:HA2 | 1:59:A:LEU:HB3 | 13       | 0.11          |
| (1,687) | 1:48:A:GLY:HA2 | 1:59:A:LEU:HB2 | 3        | 0.11          |
| (1,687) | 1:48:A:GLY:HA2 | 1:59:A:LEU:HB2 | 4        | 0.11          |
| (1,676) | 1:47:A:LEU:HA  | 1:49:A:LEU:H   | 5        | 0.11          |
| (1,676) | 1:47:A:LEU:HA  | 1:49:A:LEU:H   | 6        | 0.11          |
| (1,676) | 1:47:A:LEU:HA  | 1:49:A:LEU:H   | 7        | 0.11          |
| (1,676) | 1:47:A:LEU:HA  | 1:49:A:LEU:H   | 15       | 0.11          |
| (1,676) | 1:47:A:LEU:HA  | 1:49:A:LEU:H   | 18       | 0.11          |
| (1,675) | 1:47:A:LEU:HA  | 1:51:A:LEU:HA  | 9        | 0.11          |
| (1,674) | 1:47:A:LEU:HG  | 1:51:A:LEU:HB3 | 1        | 0.11          |
| (1,674) | 1:47:A:LEU:HG  | 1:51:A:LEU:HB3 | 6        | 0.11          |
| (1,673) | 1:47:A:LEU:HB3 | 1:51:A:LEU:HG  | 1        | 0.11          |
| (1,673) | 1:47:A:LEU:HB3 | 1:51:A:LEU:HG  | 2        | 0.11          |
| (1,673) | 1:47:A:LEU:HB3 | 1:51:A:LEU:HG  | 14       | 0.11          |
| (1,673) | 1:47:A:LEU:HB3 | 1:51:A:LEU:HG  | 15       | 0.11          |
| (1,673) | 1:47:A:LEU:HB3 | 1:51:A:LEU:HG  | 16       | 0.11          |
| (1,667) | 1:46:A:GLU:HB3 | 1:49:A:LEU:HB2 | 14       | 0.11          |
| (1,665) | 1:46:A:GLU:H   | 1:47:A:LEU:HB2 | 1        | 0.11          |
| (1,665) | 1:46:A:GLU:H   | 1:47:A:LEU:HB2 | 12       | 0.11          |
| (1,665) | 1:46:A:GLU:H   | 1:47:A:LEU:HB2 | 18       | 0.11          |
| (1,652) | 1:45:A:LEU:HA  | 1:49:A:LEU:HB3 | 4        | 0.11          |
| (1,651) | 1:45:A:LEU:HA  | 1:48:A:GLY:HA2 | 10       | 0.11          |
| (1,651) | 1:45:A:LEU:HA  | 1:48:A:GLY:HA2 | 12       | 0.11          |
| (1,648) | 1:45:A:LEU:HB2 | 1:49:A:LEU:H   | 14       | 0.11          |
| (1,647) | 1:45:A:LEU:HA  | 1:49:A:LEU:HA  | 5        | 0.11          |
| (1,647) | 1:45:A:LEU:HA  | 1:49:A:LEU:HA  | 7        | 0.11          |
| (1,631) | 1:44:A:ALA:HA  | 1:47:A:LEU:HG  | 1        | 0.11          |
| (1,631) | 1:44:A:ALA:HA  | 1:47:A:LEU:HG  | 4        | 0.11          |
| (1,631) | 1:44:A:ALA:HA  | 1:47:A:LEU:HG  | 5        | 0.11          |
| (1,631) | 1:44:A:ALA:HA  | 1:47:A:LEU:HG  | 11       | 0.11          |
| (1,631) | 1:44:A:ALA:HA  | 1:47:A:LEU:HG  | 16       | 0.11          |
| (1,629) | 1:44:A:ALA:H   | 1:47:A:LEU:HB2 | 1        | 0.11          |
| (1,629) | 1:44:A:ALA:H   | 1:47:A:LEU:HB2 | 2        | 0.11          |
| (1,629) | 1:44:A:ALA:H   | 1:47:A:LEU:HB2 | 7        | 0.11          |
| (1,629) | 1:44:A:ALA:H   | 1:47:A:LEU:HB2 | 17       | 0.11          |
| (1,629) | 1:44:A:ALA:H   | 1:47:A:LEU:HB2 | 20       | 0.11          |
| (1,628) | 1:44:A:ALA:HA  | 1:48:A:GLY:HA3 | 6        | 0.11          |
| (1,628) | 1:44:A:ALA:HA  | 1:48:A:GLY:HA3 | 10       | 0.11          |
| (1,618) | 1:43:A:ASP:HB3 | 1:46:A:GLU:H   | 13       | 0.11          |
| (1,618) | 1:43:A:ASP:HB3 | 1:46:A:GLU:H   | 20       | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,616) | 1:43:A:ASP:HA   | 1:46:A:GLU:HA   | 2        | 0.11          |
| (1,616) | 1:43:A:ASP:HA   | 1:46:A:GLU:HA   | 10       | 0.11          |
| (1,616) | 1:43:A:ASP:HA   | 1:46:A:GLU:HA   | 12       | 0.11          |
| (1,616) | 1:43:A:ASP:HA   | 1:46:A:GLU:HA   | 14       | 0.11          |
| (1,616) | 1:43:A:ASP:HA   | 1:46:A:GLU:HA   | 15       | 0.11          |
| (1,616) | 1:43:A:ASP:HA   | 1:46:A:GLU:HA   | 20       | 0.11          |
| (1,601) | 1:41:A:SER:HA   | 1:44:A:ALA:HA   | 11       | 0.11          |
| (1,600) | 1:41:A:SER:HA   | 1:45:A:LEU:H    | 5        | 0.11          |
| (1,600) | 1:41:A:SER:HA   | 1:45:A:LEU:H    | 9        | 0.11          |
| (1,572) | 1:39:A:LEU:HA   | 1:43:A:ASP:H    | 7        | 0.11          |
| (1,572) | 1:39:A:LEU:HA   | 1:43:A:ASP:H    | 9        | 0.11          |
| (1,572) | 1:39:A:LEU:HA   | 1:43:A:ASP:H    | 11       | 0.11          |
| (1,571) | 1:39:A:LEU:HB2  | 1:43:A:ASP:H    | 3        | 0.11          |
| (1,571) | 1:39:A:LEU:HB2  | 1:43:A:ASP:H    | 19       | 0.11          |
| (1,536) | 1:33:A:PHE:HE1  | 1:39:A:LEU:H    | 7        | 0.11          |
| (1,535) | 1:33:A:PHE:HA   | 1:39:A:LEU:HB3  | 10       | 0.11          |
| (1,517) | 1:32:A:LEU:HB2  | 1:39:A:LEU:H    | 3        | 0.11          |
| (1,517) | 1:32:A:LEU:HB2  | 1:39:A:LEU:H    | 20       | 0.11          |
| (1,505) | 1:31:A:PRO:HB3  | 1:34:A:GLY:HA2  | 10       | 0.11          |
| (1,480) | 1:29:A:GLU:H    | 1:74:A:GLN:HB3  | 16       | 0.11          |
| (1,479) | 1:29:A:GLU:HA   | 1:72:A:SER:H    | 4        | 0.11          |
| (1,464) | 1:28:A:THR:HG23 | 1:74:A:GLN:HA   | 9        | 0.11          |
| (1,414) | 1:21:A:ILE:HG13 | 1:25:A:ASP:HB2  | 1        | 0.11          |
| (1,414) | 1:21:A:ILE:HG13 | 1:25:A:ASP:HB2  | 12       | 0.11          |
| (1,414) | 1:21:A:ILE:HG13 | 1:25:A:ASP:HB2  | 19       | 0.11          |
| (1,406) | 1:19:A:GLU:HB3  | 1:21:A:ILE:H    | 7        | 0.11          |
| (1,388) | 1:18:A:LEU:HB3  | 1:21:A:ILE:HA   | 3        | 0.11          |
| (1,388) | 1:18:A:LEU:HB3  | 1:21:A:ILE:HA   | 7        | 0.11          |
| (1,388) | 1:18:A:LEU:HB3  | 1:21:A:ILE:HA   | 11       | 0.11          |
| (1,388) | 1:18:A:LEU:HB3  | 1:21:A:ILE:HA   | 20       | 0.11          |
| (1,387) | 1:18:A:LEU:HB2  | 1:21:A:ILE:HG12 | 18       | 0.11          |
| (1,387) | 1:18:A:LEU:HB2  | 1:21:A:ILE:HG12 | 19       | 0.11          |
| (1,362) | 1:16:A:LEU:HG   | 1:43:A:ASP:HB2  | 1        | 0.11          |
| (1,362) | 1:16:A:LEU:HG   | 1:43:A:ASP:HB2  | 12       | 0.11          |
| (1,362) | 1:16:A:LEU:HG   | 1:43:A:ASP:HB2  | 14       | 0.11          |
| (1,362) | 1:16:A:LEU:HG   | 1:43:A:ASP:HB2  | 15       | 0.11          |
| (1,360) | 1:16:A:LEU:HB2  | 1:37:A:LEU:HG   | 2        | 0.11          |
| (1,360) | 1:16:A:LEU:HB2  | 1:37:A:LEU:HG   | 4        | 0.11          |
| (1,360) | 1:16:A:LEU:HB2  | 1:37:A:LEU:HG   | 9        | 0.11          |
| (1,360) | 1:16:A:LEU:HB2  | 1:37:A:LEU:HG   | 17       | 0.11          |
| (1,357) | 1:16:A:LEU:HB2  | 1:18:A:LEU:HA   | 3        | 0.11          |
| (1,357) | 1:16:A:LEU:HB2  | 1:18:A:LEU:HA   | 12       | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,357) | 1:16:A:LEU:HB2  | 1:18:A:LEU:HA   | 18       | 0.11          |
| (1,337) | 1:15:A:VAL:HB   | 1:51:A:LEU:HG   | 5        | 0.11          |
| (1,308) | 1:13:A:ILE:HA   | 1:18:A:LEU:HA   | 2        | 0.11          |
| (1,308) | 1:13:A:ILE:HA   | 1:18:A:LEU:HA   | 8        | 0.11          |
| (1,308) | 1:13:A:ILE:HA   | 1:18:A:LEU:HA   | 11       | 0.11          |
| (1,308) | 1:13:A:ILE:HA   | 1:18:A:LEU:HA   | 19       | 0.11          |
| (1,291) | 1:12:A:ILE:HG12 | 1:47:A:LEU:HA   | 12       | 0.11          |
| (1,289) | 1:12:A:ILE:HG13 | 1:15:A:VAL:H    | 3        | 0.11          |
| (1,289) | 1:12:A:ILE:HG13 | 1:15:A:VAL:H    | 5        | 0.11          |
| (1,289) | 1:12:A:ILE:HG13 | 1:15:A:VAL:H    | 15       | 0.11          |
| (1,286) | 1:12:A:ILE:H    | 1:14:A:ASP:H    | 1        | 0.11          |
| (1,286) | 1:12:A:ILE:H    | 1:14:A:ASP:H    | 7        | 0.11          |
| (1,286) | 1:12:A:ILE:H    | 1:14:A:ASP:H    | 9        | 0.11          |
| (1,286) | 1:12:A:ILE:H    | 1:14:A:ASP:H    | 12       | 0.11          |
| (1,263) | 1:11:A:MET:HB3  | 1:15:A:VAL:H    | 2        | 0.11          |
| (1,263) | 1:11:A:MET:HB3  | 1:15:A:VAL:H    | 5        | 0.11          |
| (1,263) | 1:11:A:MET:HB3  | 1:15:A:VAL:H    | 6        | 0.11          |
| (1,263) | 1:11:A:MET:HB3  | 1:15:A:VAL:H    | 7        | 0.11          |
| (1,263) | 1:11:A:MET:HB3  | 1:15:A:VAL:H    | 8        | 0.11          |
| (1,263) | 1:11:A:MET:HB3  | 1:15:A:VAL:H    | 9        | 0.11          |
| (1,263) | 1:11:A:MET:HB3  | 1:15:A:VAL:H    | 10       | 0.11          |
| (1,263) | 1:11:A:MET:HB3  | 1:15:A:VAL:H    | 13       | 0.11          |
| (1,263) | 1:11:A:MET:HB3  | 1:15:A:VAL:H    | 14       | 0.11          |
| (1,263) | 1:11:A:MET:HB3  | 1:15:A:VAL:H    | 15       | 0.11          |
| (1,263) | 1:11:A:MET:HB3  | 1:15:A:VAL:H    | 16       | 0.11          |
| (1,263) | 1:11:A:MET:HB3  | 1:15:A:VAL:H    | 17       | 0.11          |
| (1,258) | 1:11:A:MET:HB2  | 1:15:A:VAL:HB   | 1        | 0.11          |
| (1,258) | 1:11:A:MET:HB2  | 1:15:A:VAL:HB   | 2        | 0.11          |
| (1,258) | 1:11:A:MET:HB2  | 1:15:A:VAL:HB   | 8        | 0.11          |
| (1,258) | 1:11:A:MET:HB2  | 1:15:A:VAL:HB   | 10       | 0.11          |
| (1,258) | 1:11:A:MET:HB2  | 1:15:A:VAL:HB   | 20       | 0.11          |
| (1,257) | 1:11:A:MET:HA   | 1:15:A:VAL:HA   | 9        | 0.11          |
| (1,257) | 1:11:A:MET:HA   | 1:15:A:VAL:HA   | 17       | 0.11          |
| (1,232) | 1:10:A:GLN:HG3  | 1:23:A:ILE:HG13 | 1        | 0.11          |
| (1,232) | 1:10:A:GLN:HG3  | 1:23:A:ILE:HG13 | 6        | 0.11          |
| (1,232) | 1:10:A:GLN:HG3  | 1:23:A:ILE:HG13 | 7        | 0.11          |
| (1,232) | 1:10:A:GLN:HG3  | 1:23:A:ILE:HG13 | 16       | 0.11          |
| (1,232) | 1:10:A:GLN:HG3  | 1:23:A:ILE:HG13 | 20       | 0.11          |
| (1,231) | 1:10:A:GLN:HA   | 1:12:A:ILE:HB   | 8        | 0.11          |
| (1,231) | 1:10:A:GLN:HA   | 1:12:A:ILE:HB   | 11       | 0.11          |
| (1,231) | 1:10:A:GLN:HA   | 1:12:A:ILE:HB   | 13       | 0.11          |
| (1,231) | 1:10:A:GLN:HA   | 1:12:A:ILE:HB   | 19       | 0.11          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,230) | 1:10:A:GLN:HB2 | 1:14:A:ASP:H   | 4        | 0.11          |
| (1,230) | 1:10:A:GLN:HB2 | 1:14:A:ASP:H   | 6        | 0.11          |
| (1,230) | 1:10:A:GLN:HB2 | 1:14:A:ASP:H   | 14       | 0.11          |
| (1,229) | 1:10:A:GLN:H   | 1:14:A:ASP:HB3 | 6        | 0.11          |
| (1,229) | 1:10:A:GLN:H   | 1:14:A:ASP:HB3 | 14       | 0.11          |
| (1,229) | 1:10:A:GLN:H   | 1:14:A:ASP:HB3 | 15       | 0.11          |
| (1,228) | 1:10:A:GLN:HG3 | 1:22:A:THR:HA  | 1        | 0.11          |
| (1,228) | 1:10:A:GLN:HG3 | 1:22:A:THR:HA  | 5        | 0.11          |
| (1,228) | 1:10:A:GLN:HG3 | 1:22:A:THR:HA  | 6        | 0.11          |
| (1,228) | 1:10:A:GLN:HG3 | 1:22:A:THR:HA  | 13       | 0.11          |
| (1,228) | 1:10:A:GLN:HG3 | 1:22:A:THR:HA  | 20       | 0.11          |
| (1,227) | 1:10:A:GLN:HG2 | 1:14:A:ASP:HA  | 1        | 0.11          |
| (1,227) | 1:10:A:GLN:HG2 | 1:14:A:ASP:HA  | 5        | 0.11          |
| (1,227) | 1:10:A:GLN:HG2 | 1:14:A:ASP:HA  | 7        | 0.11          |
| (1,227) | 1:10:A:GLN:HG2 | 1:14:A:ASP:HA  | 9        | 0.11          |
| (1,227) | 1:10:A:GLN:HG2 | 1:14:A:ASP:HA  | 10       | 0.11          |
| (1,227) | 1:10:A:GLN:HG2 | 1:14:A:ASP:HA  | 18       | 0.11          |
| (1,227) | 1:10:A:GLN:HG2 | 1:14:A:ASP:HA  | 19       | 0.11          |
| (1,226) | 1:10:A:GLN:HB3 | 1:14:A:ASP:H   | 4        | 0.11          |
| (1,226) | 1:10:A:GLN:HB3 | 1:14:A:ASP:H   | 6        | 0.11          |
| (1,226) | 1:10:A:GLN:HB3 | 1:14:A:ASP:H   | 9        | 0.11          |
| (1,226) | 1:10:A:GLN:HB3 | 1:14:A:ASP:H   | 15       | 0.11          |
| (1,226) | 1:10:A:GLN:HB3 | 1:14:A:ASP:H   | 19       | 0.11          |
| (1,226) | 1:10:A:GLN:HB3 | 1:14:A:ASP:H   | 20       | 0.11          |
| (1,225) | 1:10:A:GLN:HA  | 1:13:A:ILE:HA  | 5        | 0.11          |
| (1,225) | 1:10:A:GLN:HA  | 1:13:A:ILE:HA  | 7        | 0.11          |
| (1,225) | 1:10:A:GLN:HA  | 1:13:A:ILE:HA  | 8        | 0.11          |
| (1,225) | 1:10:A:GLN:HA  | 1:13:A:ILE:HA  | 12       | 0.11          |
| (1,225) | 1:10:A:GLN:HA  | 1:13:A:ILE:HA  | 14       | 0.11          |
| (1,225) | 1:10:A:GLN:HA  | 1:13:A:ILE:HA  | 17       | 0.11          |
| (1,224) | 1:10:A:GLN:H   | 1:12:A:ILE:HA  | 1        | 0.11          |
| (1,224) | 1:10:A:GLN:H   | 1:12:A:ILE:HA  | 12       | 0.11          |
| (1,224) | 1:10:A:GLN:H   | 1:12:A:ILE:HA  | 18       | 0.11          |
| (1,223) | 1:10:A:GLN:HB2 | 1:22:A:THR:HB  | 3        | 0.11          |
| (1,223) | 1:10:A:GLN:HB2 | 1:22:A:THR:HB  | 7        | 0.11          |
| (1,223) | 1:10:A:GLN:HB2 | 1:22:A:THR:HB  | 10       | 0.11          |
| (1,223) | 1:10:A:GLN:HB2 | 1:22:A:THR:HB  | 11       | 0.11          |
| (1,223) | 1:10:A:GLN:HB2 | 1:22:A:THR:HB  | 12       | 0.11          |
| (1,223) | 1:10:A:GLN:HB2 | 1:22:A:THR:HB  | 13       | 0.11          |
| (1,223) | 1:10:A:GLN:HB2 | 1:22:A:THR:HB  | 17       | 0.11          |
| (1,223) | 1:10:A:GLN:HB2 | 1:22:A:THR:HB  | 19       | 0.11          |
| (1,193) | 1:9:A:LYS:HA   | 1:26:A:ILE:HB  | 4        | 0.11          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,191) | 1:9:A:LYS:HA  | 1:13:A:ILE:HA   | 3        | 0.11          |
| (1,191) | 1:9:A:LYS:HA  | 1:13:A:ILE:HA   | 4        | 0.11          |
| (1,190) | 1:9:A:LYS:HA  | 1:73:A:ILE:HB   | 5        | 0.11          |
| (1,187) | 1:9:A:LYS:H   | 1:12:A:ILE:HB   | 7        | 0.11          |
| (1,187) | 1:9:A:LYS:H   | 1:12:A:ILE:HB   | 10       | 0.11          |
| (1,187) | 1:9:A:LYS:H   | 1:12:A:ILE:HB   | 18       | 0.11          |
| (1,186) | 1:9:A:LYS:H   | 1:11:A:MET:HB2  | 5        | 0.11          |
| (1,186) | 1:9:A:LYS:H   | 1:11:A:MET:HB2  | 6        | 0.11          |
| (1,186) | 1:9:A:LYS:H   | 1:11:A:MET:HB2  | 10       | 0.11          |
| (1,186) | 1:9:A:LYS:H   | 1:11:A:MET:HB2  | 11       | 0.11          |
| (1,186) | 1:9:A:LYS:H   | 1:11:A:MET:HB2  | 16       | 0.11          |
| (1,186) | 1:9:A:LYS:H   | 1:11:A:MET:HB2  | 20       | 0.11          |
| (1,185) | 1:9:A:LYS:HB3 | 1:12:A:ILE:H    | 1        | 0.11          |
| (1,185) | 1:9:A:LYS:HB3 | 1:12:A:ILE:H    | 4        | 0.11          |
| (1,185) | 1:9:A:LYS:HB3 | 1:12:A:ILE:H    | 5        | 0.11          |
| (1,185) | 1:9:A:LYS:HB3 | 1:12:A:ILE:H    | 12       | 0.11          |
| (1,185) | 1:9:A:LYS:HB3 | 1:12:A:ILE:H    | 16       | 0.11          |
| (1,185) | 1:9:A:LYS:HB3 | 1:12:A:ILE:H    | 18       | 0.11          |
| (1,184) | 1:9:A:LYS:HB2 | 1:13:A:ILE:HG13 | 6        | 0.11          |
| (1,184) | 1:9:A:LYS:HB2 | 1:13:A:ILE:HG13 | 7        | 0.11          |
| (1,184) | 1:9:A:LYS:HB2 | 1:13:A:ILE:HG13 | 12       | 0.11          |
| (1,184) | 1:9:A:LYS:HB2 | 1:13:A:ILE:HG13 | 13       | 0.11          |
| (1,184) | 1:9:A:LYS:HB2 | 1:13:A:ILE:HG13 | 14       | 0.11          |
| (1,184) | 1:9:A:LYS:HB2 | 1:13:A:ILE:HG13 | 17       | 0.11          |
| (1,183) | 1:9:A:LYS:HB2 | 1:13:A:ILE:H    | 4        | 0.11          |
| (1,183) | 1:9:A:LYS:HB2 | 1:13:A:ILE:H    | 6        | 0.11          |
| (1,183) | 1:9:A:LYS:HB2 | 1:13:A:ILE:H    | 7        | 0.11          |
| (1,183) | 1:9:A:LYS:HB2 | 1:13:A:ILE:H    | 8        | 0.11          |
| (1,183) | 1:9:A:LYS:HB2 | 1:13:A:ILE:H    | 11       | 0.11          |
| (1,183) | 1:9:A:LYS:HB2 | 1:13:A:ILE:H    | 12       | 0.11          |
| (1,183) | 1:9:A:LYS:HB2 | 1:13:A:ILE:H    | 13       | 0.11          |
| (1,183) | 1:9:A:LYS:HB2 | 1:13:A:ILE:H    | 17       | 0.11          |
| (1,183) | 1:9:A:LYS:HB2 | 1:13:A:ILE:H    | 18       | 0.11          |
| (1,183) | 1:9:A:LYS:HB2 | 1:13:A:ILE:H    | 20       | 0.11          |
| (1,182) | 1:9:A:LYS:HA  | 1:13:A:ILE:HB   | 3        | 0.11          |
| (1,182) | 1:9:A:LYS:HA  | 1:13:A:ILE:HB   | 6        | 0.11          |
| (1,182) | 1:9:A:LYS:HA  | 1:13:A:ILE:HB   | 10       | 0.11          |
| (1,182) | 1:9:A:LYS:HA  | 1:13:A:ILE:HB   | 20       | 0.11          |
| (1,143) | 1:8:A:LEU:HA  | 1:12:A:ILE:HA   | 1        | 0.11          |
| (1,143) | 1:8:A:LEU:HA  | 1:12:A:ILE:HA   | 2        | 0.11          |
| (1,143) | 1:8:A:LEU:HA  | 1:12:A:ILE:HA   | 6        | 0.11          |
| (1,143) | 1:8:A:LEU:HA  | 1:12:A:ILE:HA   | 7        | 0.11          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,143) | 1:8:A:LEU:HA  | 1:12:A:ILE:HA   | 8        | 0.11          |
| (1,143) | 1:8:A:LEU:HA  | 1:12:A:ILE:HA   | 9        | 0.11          |
| (1,143) | 1:8:A:LEU:HA  | 1:12:A:ILE:HA   | 11       | 0.11          |
| (1,143) | 1:8:A:LEU:HA  | 1:12:A:ILE:HA   | 15       | 0.11          |
| (1,143) | 1:8:A:LEU:HA  | 1:12:A:ILE:HA   | 18       | 0.11          |
| (1,142) | 1:8:A:LEU:HA  | 1:11:A:MET:HA   | 6        | 0.11          |
| (1,142) | 1:8:A:LEU:HA  | 1:11:A:MET:HA   | 14       | 0.11          |
| (1,142) | 1:8:A:LEU:HA  | 1:11:A:MET:HA   | 17       | 0.11          |
| (1,138) | 1:8:A:LEU:HB2 | 1:11:A:MET:H    | 1        | 0.11          |
| (1,138) | 1:8:A:LEU:HB2 | 1:11:A:MET:H    | 8        | 0.11          |
| (1,138) | 1:8:A:LEU:HB2 | 1:11:A:MET:H    | 9        | 0.11          |
| (1,138) | 1:8:A:LEU:HB2 | 1:11:A:MET:H    | 18       | 0.11          |
| (1,137) | 1:8:A:LEU:HA  | 1:76:A:LEU:HB2  | 5        | 0.11          |
| (1,137) | 1:8:A:LEU:HA  | 1:76:A:LEU:HB2  | 19       | 0.11          |
| (1,137) | 1:8:A:LEU:HA  | 1:76:A:LEU:HB2  | 20       | 0.11          |
| (1,136) | 1:8:A:LEU:HB3 | 1:12:A:ILE:HA   | 1        | 0.11          |
| (1,136) | 1:8:A:LEU:HB3 | 1:12:A:ILE:HA   | 3        | 0.11          |
| (1,136) | 1:8:A:LEU:HB3 | 1:12:A:ILE:HA   | 5        | 0.11          |
| (1,136) | 1:8:A:LEU:HB3 | 1:12:A:ILE:HA   | 13       | 0.11          |
| (1,136) | 1:8:A:LEU:HB3 | 1:12:A:ILE:HA   | 17       | 0.11          |
| (1,136) | 1:8:A:LEU:HB3 | 1:12:A:ILE:HA   | 20       | 0.11          |
| (1,133) | 1:8:A:LEU:HB2 | 1:12:A:ILE:HG13 | 3        | 0.11          |
| (1,133) | 1:8:A:LEU:HB2 | 1:12:A:ILE:HG13 | 4        | 0.11          |
| (1,133) | 1:8:A:LEU:HB2 | 1:12:A:ILE:HG13 | 5        | 0.11          |
| (1,133) | 1:8:A:LEU:HB2 | 1:12:A:ILE:HG13 | 9        | 0.11          |
| (1,133) | 1:8:A:LEU:HB2 | 1:12:A:ILE:HG13 | 13       | 0.11          |
| (1,133) | 1:8:A:LEU:HB2 | 1:12:A:ILE:HG13 | 17       | 0.11          |
| (1,131) | 1:8:A:LEU:HA  | 1:12:A:ILE:HG12 | 2        | 0.11          |
| (1,131) | 1:8:A:LEU:HA  | 1:12:A:ILE:HG12 | 3        | 0.11          |
| (1,131) | 1:8:A:LEU:HA  | 1:12:A:ILE:HG12 | 7        | 0.11          |
| (1,131) | 1:8:A:LEU:HA  | 1:12:A:ILE:HG12 | 10       | 0.11          |
| (1,131) | 1:8:A:LEU:HA  | 1:12:A:ILE:HG12 | 13       | 0.11          |
| (1,131) | 1:8:A:LEU:HA  | 1:12:A:ILE:HG12 | 14       | 0.11          |
| (1,131) | 1:8:A:LEU:HA  | 1:12:A:ILE:HG12 | 15       | 0.11          |
| (1,131) | 1:8:A:LEU:HA  | 1:12:A:ILE:HG12 | 19       | 0.11          |
| (1,128) | 1:8:A:LEU:HA  | 1:76:A:LEU:HB3  | 1        | 0.11          |
| (1,128) | 1:8:A:LEU:HA  | 1:76:A:LEU:HB3  | 7        | 0.11          |
| (1,128) | 1:8:A:LEU:HA  | 1:76:A:LEU:HB3  | 10       | 0.11          |
| (1,128) | 1:8:A:LEU:HA  | 1:76:A:LEU:HB3  | 14       | 0.11          |
| (1,128) | 1:8:A:LEU:HA  | 1:76:A:LEU:HB3  | 18       | 0.11          |
| (1,127) | 1:8:A:LEU:HA  | 1:12:A:ILE:HB   | 2        | 0.11          |
| (1,127) | 1:8:A:LEU:HA  | 1:12:A:ILE:HB   | 6        | 0.11          |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,127) | 1:8:A:LEU:HA  | 1:12:A:ILE:HB   | 7        | 0.11          |
| (1,127) | 1:8:A:LEU:HA  | 1:12:A:ILE:HB   | 13       | 0.11          |
| (1,127) | 1:8:A:LEU:HA  | 1:12:A:ILE:HB   | 14       | 0.11          |
| (1,127) | 1:8:A:LEU:HA  | 1:12:A:ILE:HB   | 15       | 0.11          |
| (1,127) | 1:8:A:LEU:HA  | 1:12:A:ILE:HB   | 19       | 0.11          |
| (1,127) | 1:8:A:LEU:HA  | 1:12:A:ILE:HB   | 20       | 0.11          |
| (1,125) | 1:8:A:LEU:HB3 | 1:77:A:VAL:HA   | 2        | 0.11          |
| (1,125) | 1:8:A:LEU:HB3 | 1:77:A:VAL:HA   | 17       | 0.11          |
| (1,125) | 1:8:A:LEU:HB3 | 1:77:A:VAL:HA   | 19       | 0.11          |
| (1,113) | 1:7:A:GLU:HA  | 1:11:A:MET:HB3  | 5        | 0.11          |
| (1,113) | 1:7:A:GLU:HA  | 1:11:A:MET:HB3  | 8        | 0.11          |
| (1,113) | 1:7:A:GLU:HA  | 1:11:A:MET:HB3  | 9        | 0.11          |
| (1,113) | 1:7:A:GLU:HA  | 1:11:A:MET:HB3  | 11       | 0.11          |
| (1,113) | 1:7:A:GLU:HA  | 1:11:A:MET:HB3  | 14       | 0.11          |
| (1,112) | 1:7:A:GLU:HB3 | 1:10:A:GLN:HB2  | 3        | 0.11          |
| (1,112) | 1:7:A:GLU:HB3 | 1:10:A:GLN:HB2  | 5        | 0.11          |
| (1,112) | 1:7:A:GLU:HB3 | 1:10:A:GLN:HB2  | 6        | 0.11          |
| (1,112) | 1:7:A:GLU:HB3 | 1:10:A:GLN:HB2  | 10       | 0.11          |
| (1,112) | 1:7:A:GLU:HB3 | 1:10:A:GLN:HB2  | 11       | 0.11          |
| (1,112) | 1:7:A:GLU:HB3 | 1:10:A:GLN:HB2  | 13       | 0.11          |
| (1,112) | 1:7:A:GLU:HB3 | 1:10:A:GLN:HB2  | 15       | 0.11          |
| (1,112) | 1:7:A:GLU:HB3 | 1:10:A:GLN:HB2  | 17       | 0.11          |
| (1,112) | 1:7:A:GLU:HB3 | 1:10:A:GLN:HB2  | 18       | 0.11          |
| (1,112) | 1:7:A:GLU:HB3 | 1:10:A:GLN:HB2  | 20       | 0.11          |
| (1,111) | 1:7:A:GLU:H   | 1:10:A:GLN:HB2  | 1        | 0.11          |
| (1,111) | 1:7:A:GLU:H   | 1:10:A:GLN:HB2  | 2        | 0.11          |
| (1,111) | 1:7:A:GLU:H   | 1:10:A:GLN:HB2  | 11       | 0.11          |
| (1,111) | 1:7:A:GLU:H   | 1:10:A:GLN:HB2  | 14       | 0.11          |
| (1,70)  | 1:5:A:ALA:H   | 1:77:A:VAL:HA   | 1        | 0.11          |
| (1,68)  | 1:5:A:ALA:HA  | 1:9:A:LYS:HB2   | 14       | 0.11          |
| (1,68)  | 1:5:A:ALA:HA  | 1:9:A:LYS:HB2   | 20       | 0.11          |
| (1,66)  | 1:5:A:ALA:HA  | 1:73:A:ILE:HG13 | 1        | 0.11          |
| (1,66)  | 1:5:A:ALA:HA  | 1:73:A:ILE:HG13 | 16       | 0.11          |
| (1,27)  | 1:4:A:LEU:HB2 | 1:84:A:GLN:HG3  | 6        | 0.11          |
| (1,27)  | 1:4:A:LEU:HB2 | 1:84:A:GLN:HG3  | 10       | 0.11          |
| (1,27)  | 1:4:A:LEU:HB2 | 1:84:A:GLN:HG3  | 12       | 0.11          |
| (1,27)  | 1:4:A:LEU:HB2 | 1:84:A:GLN:HG3  | 13       | 0.11          |
| (1,27)  | 1:4:A:LEU:HB2 | 1:84:A:GLN:HG3  | 14       | 0.11          |
| (1,27)  | 1:4:A:LEU:HB2 | 1:84:A:GLN:HG3  | 19       | 0.11          |
| (1,26)  | 1:4:A:LEU:HB3 | 1:81:A:GLU:HA   | 3        | 0.11          |
| (1,23)  | 1:4:A:LEU:HA  | 1:8:A:LEU:HB2   | 1        | 0.11          |
| (1,23)  | 1:4:A:LEU:HA  | 1:8:A:LEU:HB2   | 3        | 0.11          |

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| Key    | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|--------|---------------|---------------|----------|---------------|
| (1,23) | 1:4:A:LEU:HA  | 1:8:A:LEU:HB2 | 7        | 0.11          |
| (1,23) | 1:4:A:LEU:HA  | 1:8:A:LEU:HB2 | 8        | 0.11          |
| (1,23) | 1:4:A:LEU:HA  | 1:8:A:LEU:HB2 | 10       | 0.11          |
| (1,23) | 1:4:A:LEU:HA  | 1:8:A:LEU:HB2 | 15       | 0.11          |
| (1,23) | 1:4:A:LEU:HA  | 1:8:A:LEU:HB2 | 18       | 0.11          |
| (1,22) | 1:4:A:LEU:HB2 | 1:77:A:VAL:HA | 9        | 0.11          |
| (1,22) | 1:4:A:LEU:HB2 | 1:77:A:VAL:HA | 14       | 0.11          |
| (1,22) | 1:4:A:LEU:HB2 | 1:77:A:VAL:HA | 17       | 0.11          |
| (1,19) | 1:4:A:LEU:HG  | 1:81:A:GLU:HA | 2        | 0.11          |
| (1,19) | 1:4:A:LEU:HG  | 1:81:A:GLU:HA | 8        | 0.11          |
| (1,19) | 1:4:A:LEU:HG  | 1:81:A:GLU:HA | 13       | 0.11          |
| (1,18) | 1:4:A:LEU:HA  | 1:8:A:LEU:HA  | 1        | 0.11          |
| (1,18) | 1:4:A:LEU:HA  | 1:8:A:LEU:HA  | 3        | 0.11          |
| (1,18) | 1:4:A:LEU:HA  | 1:8:A:LEU:HA  | 5        | 0.11          |
| (1,18) | 1:4:A:LEU:HA  | 1:8:A:LEU:HA  | 7        | 0.11          |
| (1,18) | 1:4:A:LEU:HA  | 1:8:A:LEU:HA  | 9        | 0.11          |
| (1,18) | 1:4:A:LEU:HA  | 1:8:A:LEU:HA  | 11       | 0.11          |
| (1,18) | 1:4:A:LEU:HA  | 1:8:A:LEU:HA  | 14       | 0.11          |
| (1,18) | 1:4:A:LEU:HA  | 1:8:A:LEU:HA  | 17       | 0.11          |
| (1,16) | 1:4:A:LEU:HB2 | 1:77:A:VAL:HB | 5        | 0.11          |
| (1,16) | 1:4:A:LEU:HB2 | 1:77:A:VAL:HB | 6        | 0.11          |
| (1,16) | 1:4:A:LEU:HB2 | 1:77:A:VAL:HB | 10       | 0.11          |
| (1,16) | 1:4:A:LEU:HB2 | 1:77:A:VAL:HB | 11       | 0.11          |
| (1,16) | 1:4:A:LEU:HB2 | 1:77:A:VAL:HB | 12       | 0.11          |
| (1,16) | 1:4:A:LEU:HB2 | 1:77:A:VAL:HB | 14       | 0.11          |
| (1,15) | 1:4:A:LEU:HG  | 1:7:A:GLU:HB2 | 1        | 0.11          |
| (1,15) | 1:4:A:LEU:HG  | 1:7:A:GLU:HB2 | 3        | 0.11          |
| (1,15) | 1:4:A:LEU:HG  | 1:7:A:GLU:HB2 | 7        | 0.11          |
| (1,15) | 1:4:A:LEU:HG  | 1:7:A:GLU:HB2 | 8        | 0.11          |
| (1,14) | 1:4:A:LEU:HB2 | 1:8:A:LEU:HB2 | 1        | 0.11          |
| (1,14) | 1:4:A:LEU:HB2 | 1:8:A:LEU:HB2 | 2        | 0.11          |
| (1,14) | 1:4:A:LEU:HB2 | 1:8:A:LEU:HB2 | 3        | 0.11          |
| (1,14) | 1:4:A:LEU:HB2 | 1:8:A:LEU:HB2 | 4        | 0.11          |
| (1,14) | 1:4:A:LEU:HB2 | 1:8:A:LEU:HB2 | 5        | 0.11          |
| (1,14) | 1:4:A:LEU:HB2 | 1:8:A:LEU:HB2 | 11       | 0.11          |
| (1,14) | 1:4:A:LEU:HB2 | 1:8:A:LEU:HB2 | 12       | 0.11          |
| (1,14) | 1:4:A:LEU:HB2 | 1:8:A:LEU:HB2 | 14       | 0.11          |
| (1,14) | 1:4:A:LEU:HB2 | 1:8:A:LEU:HB2 | 16       | 0.11          |
| (1,14) | 1:4:A:LEU:HB2 | 1:8:A:LEU:HB2 | 17       | 0.11          |
| (1,14) | 1:4:A:LEU:HB2 | 1:8:A:LEU:HB2 | 19       | 0.11          |
| (1,13) | 1:4:A:LEU:HG  | 1:8:A:LEU:HA  | 1        | 0.11          |
| (1,13) | 1:4:A:LEU:HG  | 1:8:A:LEU:HA  | 12       | 0.11          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,12)   | 1:4:A:LEU:HA   | 1:7:A:GLU:HA    | 15       | 0.11          |
| (1,12)   | 1:4:A:LEU:HA   | 1:7:A:GLU:HA    | 17       | 0.11          |
| (1,7)    | 1:3:A:ASN:H    | 1:84:A:GLN:HE22 | 2        | 0.11          |
| (1,7)    | 1:3:A:ASN:H    | 1:84:A:GLN:HE22 | 5        | 0.11          |
| (1,7)    | 1:3:A:ASN:H    | 1:84:A:GLN:HE22 | 14       | 0.11          |
| (1,7)    | 1:3:A:ASN:H    | 1:84:A:GLN:HE22 | 17       | 0.11          |
| (2,73)   | 1:79:A:LEU:O   | 1:83:A:GLN:H    | 14       | 0.1           |
| (2,73)   | 1:79:A:LEU:O   | 1:83:A:GLN:H    | 19       | 0.1           |
| (2,71)   | 1:78:A:ALA:O   | 1:82:A:ALA:H    | 1        | 0.1           |
| (2,71)   | 1:78:A:ALA:O   | 1:82:A:ALA:H    | 3        | 0.1           |
| (2,71)   | 1:78:A:ALA:O   | 1:82:A:ALA:H    | 5        | 0.1           |
| (2,71)   | 1:78:A:ALA:O   | 1:82:A:ALA:H    | 9        | 0.1           |
| (2,71)   | 1:78:A:ALA:O   | 1:82:A:ALA:H    | 16       | 0.1           |
| (2,58)   | 1:66:A:THR:O   | 1:70:A:PHE:N    | 1        | 0.1           |
| (2,55)   | 1:65:A:GLU:O   | 1:69:A:HIS:H    | 7        | 0.1           |
| (2,55)   | 1:65:A:GLU:O   | 1:69:A:HIS:H    | 19       | 0.1           |
| (2,51)   | 1:63:A:SER:O   | 1:67:A:LYS:H    | 1        | 0.1           |
| (2,40)   | 1:47:A:LEU:O   | 1:51:A:LEU:N    | 4        | 0.1           |
| (2,40)   | 1:47:A:LEU:O   | 1:51:A:LEU:N    | 14       | 0.1           |
| (2,40)   | 1:47:A:LEU:O   | 1:51:A:LEU:N    | 20       | 0.1           |
| (2,15)   | 1:11:A:MET:O   | 1:15:A:VAL:N    | 19       | 0.1           |
| (2,9)    | 1:8:A:LEU:O    | 1:12:A:ILE:N    | 2        | 0.1           |
| (2,8)    | 1:7:A:GLU:O    | 1:11:A:MET:N    | 1        | 0.1           |
| (2,8)    | 1:7:A:GLU:O    | 1:11:A:MET:N    | 5        | 0.1           |
| (2,8)    | 1:7:A:GLU:O    | 1:11:A:MET:N    | 8        | 0.1           |
| (2,8)    | 1:7:A:GLU:O    | 1:11:A:MET:N    | 9        | 0.1           |
| (2,8)    | 1:7:A:GLU:O    | 1:11:A:MET:N    | 14       | 0.1           |
| (2,1)    | 1:4:A:LEU:O    | 1:8:A:LEU:N     | 2        | 0.1           |
| (2,1)    | 1:4:A:LEU:O    | 1:8:A:LEU:N     | 4        | 0.1           |
| (2,1)    | 1:4:A:LEU:O    | 1:8:A:LEU:N     | 8        | 0.1           |
| (2,1)    | 1:4:A:LEU:O    | 1:8:A:LEU:N     | 15       | 0.1           |
| (2,1)    | 1:4:A:LEU:O    | 1:8:A:LEU:N     | 18       | 0.1           |
| (2,1)    | 1:4:A:LEU:O    | 1:8:A:LEU:N     | 19       | 0.1           |
| (1,1227) | 1:84:A:GLN:H   | 1:85:A:LYS:HB2  | 17       | 0.1           |
| (1,1221) | 1:83:A:GLN:HB3 | 1:84:A:GLN:H    | 10       | 0.1           |
| (1,1221) | 1:83:A:GLN:HB3 | 1:84:A:GLN:H    | 11       | 0.1           |
| (1,1221) | 1:83:A:GLN:HB3 | 1:84:A:GLN:H    | 12       | 0.1           |
| (1,1217) | 1:83:A:GLN:H   | 1:85:A:LYS:H    | 4        | 0.1           |
| (1,1217) | 1:83:A:GLN:H   | 1:85:A:LYS:H    | 15       | 0.1           |
| (1,1213) | 1:82:A:ALA:HA  | 1:84:A:GLN:H    | 17       | 0.1           |
| (1,1169) | 1:80:A:VAL:HB  | 1:84:A:GLN:HG2  | 5        | 0.1           |
| (1,1168) | 1:80:A:VAL:HA  | 1:83:A:GLN:HA   | 10       | 0.1           |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1158) | 1:79:A:LEU:HB3  | 1:82:A:ALA:H   | 17       | 0.1           |
| (1,1157) | 1:79:A:LEU:H    | 1:81:A:GLU:H   | 12       | 0.1           |
| (1,1156) | 1:79:A:LEU:HB2  | 1:82:A:ALA:H   | 16       | 0.1           |
| (1,1149) | 1:78:A:ALA:H    | 1:82:A:ALA:H   | 3        | 0.1           |
| (1,1149) | 1:78:A:ALA:H    | 1:82:A:ALA:H   | 6        | 0.1           |
| (1,1149) | 1:78:A:ALA:H    | 1:82:A:ALA:H   | 11       | 0.1           |
| (1,1149) | 1:78:A:ALA:H    | 1:82:A:ALA:H   | 13       | 0.1           |
| (1,1149) | 1:78:A:ALA:H    | 1:82:A:ALA:H   | 16       | 0.1           |
| (1,1149) | 1:78:A:ALA:H    | 1:82:A:ALA:H   | 17       | 0.1           |
| (1,1149) | 1:78:A:ALA:H    | 1:82:A:ALA:H   | 20       | 0.1           |
| (1,1145) | 1:78:A:ALA:H    | 1:80:A:VAL:H   | 13       | 0.1           |
| (1,1145) | 1:78:A:ALA:H    | 1:80:A:VAL:H   | 16       | 0.1           |
| (1,1121) | 1:77:A:VAL:HA   | 1:80:A:VAL:HA  | 4        | 0.1           |
| (1,1121) | 1:77:A:VAL:HA   | 1:80:A:VAL:HA  | 15       | 0.1           |
| (1,1118) | 1:77:A:VAL:HB   | 1:81:A:GLU:H   | 17       | 0.1           |
| (1,1113) | 1:77:A:VAL:HB   | 1:79:A:LEU:H   | 2        | 0.1           |
| (1,1113) | 1:77:A:VAL:HB   | 1:79:A:LEU:H   | 4        | 0.1           |
| (1,1113) | 1:77:A:VAL:HB   | 1:79:A:LEU:H   | 13       | 0.1           |
| (1,1113) | 1:77:A:VAL:HB   | 1:79:A:LEU:H   | 18       | 0.1           |
| (1,1094) | 1:76:A:LEU:HB3  | 1:79:A:LEU:H   | 8        | 0.1           |
| (1,1094) | 1:76:A:LEU:HB3  | 1:79:A:LEU:H   | 9        | 0.1           |
| (1,1094) | 1:76:A:LEU:HB3  | 1:79:A:LEU:H   | 10       | 0.1           |
| (1,1094) | 1:76:A:LEU:HB3  | 1:79:A:LEU:H   | 16       | 0.1           |
| (1,1094) | 1:76:A:LEU:HB3  | 1:79:A:LEU:H   | 17       | 0.1           |
| (1,1091) | 1:76:A:LEU:HG   | 1:79:A:LEU:HB2 | 2        | 0.1           |
| (1,1091) | 1:76:A:LEU:HG   | 1:79:A:LEU:HB2 | 13       | 0.1           |
| (1,1080) | 1:75:A:SER:HB3  | 1:79:A:LEU:HG  | 1        | 0.1           |
| (1,1080) | 1:75:A:SER:HB3  | 1:79:A:LEU:HG  | 6        | 0.1           |
| (1,1080) | 1:75:A:SER:HB3  | 1:79:A:LEU:HG  | 11       | 0.1           |
| (1,1080) | 1:75:A:SER:HB3  | 1:79:A:LEU:HG  | 13       | 0.1           |
| (1,1080) | 1:75:A:SER:HB3  | 1:79:A:LEU:HG  | 17       | 0.1           |
| (1,1078) | 1:75:A:SER:HB2  | 1:79:A:LEU:H   | 6        | 0.1           |
| (1,1078) | 1:75:A:SER:HB2  | 1:79:A:LEU:H   | 16       | 0.1           |
| (1,1064) | 1:74:A:GLN:H    | 1:77:A:VAL:HB  | 6        | 0.1           |
| (1,1064) | 1:74:A:GLN:H    | 1:77:A:VAL:HB  | 16       | 0.1           |
| (1,1064) | 1:74:A:GLN:H    | 1:77:A:VAL:HB  | 17       | 0.1           |
| (1,1039) | 1:73:A:ILE:HB   | 1:76:A:LEU:HG  | 10       | 0.1           |
| (1,1039) | 1:73:A:ILE:HB   | 1:76:A:LEU:HG  | 18       | 0.1           |
| (1,1035) | 1:73:A:ILE:HG12 | 1:76:A:LEU:HB2 | 9        | 0.1           |
| (1,1033) | 1:73:A:ILE:HA   | 1:77:A:VAL:HA  | 3        | 0.1           |
| (1,1033) | 1:73:A:ILE:HA   | 1:77:A:VAL:HA  | 10       | 0.1           |
| (1,1033) | 1:73:A:ILE:HA   | 1:77:A:VAL:HA  | 17       | 0.1           |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1033) | 1:73:A:ILE:HA  | 1:77:A:VAL:HA  | 19       | 0.1           |
| (1,1032) | 1:73:A:ILE:H   | 1:76:A:LEU:HG  | 6        | 0.1           |
| (1,1032) | 1:73:A:ILE:H   | 1:76:A:LEU:HG  | 7        | 0.1           |
| (1,1032) | 1:73:A:ILE:H   | 1:76:A:LEU:HG  | 17       | 0.1           |
| (1,988)  | 1:70:A:PHE:HB2 | 1:76:A:LEU:HG  | 1        | 0.1           |
| (1,988)  | 1:70:A:PHE:HB2 | 1:76:A:LEU:HG  | 3        | 0.1           |
| (1,988)  | 1:70:A:PHE:HB2 | 1:76:A:LEU:HG  | 5        | 0.1           |
| (1,988)  | 1:70:A:PHE:HB2 | 1:76:A:LEU:HG  | 10       | 0.1           |
| (1,988)  | 1:70:A:PHE:HB2 | 1:76:A:LEU:HG  | 12       | 0.1           |
| (1,988)  | 1:70:A:PHE:HB2 | 1:76:A:LEU:HG  | 18       | 0.1           |
| (1,985)  | 1:70:A:PHE:HB2 | 1:75:A:SER:HB2 | 1        | 0.1           |
| (1,985)  | 1:70:A:PHE:HB2 | 1:75:A:SER:HB2 | 12       | 0.1           |
| (1,963)  | 1:69:A:HIS:HA  | 1:76:A:LEU:HA  | 13       | 0.1           |
| (1,963)  | 1:69:A:HIS:HA  | 1:76:A:LEU:HA  | 16       | 0.1           |
| (1,961)  | 1:69:A:HIS:H   | 1:75:A:SER:HB2 | 19       | 0.1           |
| (1,951)  | 1:67:A:LYS:HA  | 1:71:A:LYS:H   | 1        | 0.1           |
| (1,951)  | 1:67:A:LYS:HA  | 1:71:A:LYS:H   | 6        | 0.1           |
| (1,943)  | 1:66:A:THR:HB  | 1:69:A:HIS:H   | 5        | 0.1           |
| (1,942)  | 1:66:A:THR:HB  | 1:68:A:GLN:H   | 9        | 0.1           |
| (1,942)  | 1:66:A:THR:HB  | 1:68:A:GLN:H   | 10       | 0.1           |
| (1,942)  | 1:66:A:THR:HB  | 1:68:A:GLN:H   | 20       | 0.1           |
| (1,941)  | 1:66:A:THR:H   | 1:68:A:GLN:HG2 | 6        | 0.1           |
| (1,941)  | 1:66:A:THR:H   | 1:68:A:GLN:HG2 | 8        | 0.1           |
| (1,941)  | 1:66:A:THR:H   | 1:68:A:GLN:HG2 | 9        | 0.1           |
| (1,940)  | 1:66:A:THR:H   | 1:70:A:PHE:H   | 2        | 0.1           |
| (1,940)  | 1:66:A:THR:H   | 1:70:A:PHE:H   | 14       | 0.1           |
| (1,939)  | 1:66:A:THR:H   | 1:68:A:GLN:H   | 8        | 0.1           |
| (1,939)  | 1:66:A:THR:H   | 1:68:A:GLN:H   | 11       | 0.1           |
| (1,939)  | 1:66:A:THR:H   | 1:68:A:GLN:H   | 16       | 0.1           |
| (1,939)  | 1:66:A:THR:H   | 1:68:A:GLN:H   | 18       | 0.1           |
| (1,938)  | 1:66:A:THR:H   | 1:69:A:HIS:H   | 1        | 0.1           |
| (1,938)  | 1:66:A:THR:H   | 1:69:A:HIS:H   | 3        | 0.1           |
| (1,938)  | 1:66:A:THR:H   | 1:69:A:HIS:H   | 7        | 0.1           |
| (1,938)  | 1:66:A:THR:H   | 1:69:A:HIS:H   | 16       | 0.1           |
| (1,938)  | 1:66:A:THR:H   | 1:69:A:HIS:H   | 20       | 0.1           |
| (1,937)  | 1:66:A:THR:H   | 1:68:A:GLN:HG3 | 6        | 0.1           |
| (1,937)  | 1:66:A:THR:H   | 1:68:A:GLN:HG3 | 7        | 0.1           |
| (1,937)  | 1:66:A:THR:H   | 1:68:A:GLN:HG3 | 10       | 0.1           |
| (1,937)  | 1:66:A:THR:H   | 1:68:A:GLN:HG3 | 17       | 0.1           |
| (1,917)  | 1:65:A:GLU:HA  | 1:68:A:GLN:HA  | 5        | 0.1           |
| (1,905)  | 1:64:A:ASP:HA  | 1:67:A:LYS:HA  | 2        | 0.1           |
| (1,903)  | 1:64:A:ASP:H   | 1:67:A:LYS:H   | 6        | 0.1           |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,903) | 1:64:A:ASP:H   | 1:67:A:LYS:H   | 12       | 0.1           |
| (1,903) | 1:64:A:ASP:H   | 1:67:A:LYS:H   | 18       | 0.1           |
| (1,897) | 1:64:A:ASP:H   | 1:68:A:GLN:H   | 6        | 0.1           |
| (1,897) | 1:64:A:ASP:H   | 1:68:A:GLN:H   | 9        | 0.1           |
| (1,897) | 1:64:A:ASP:H   | 1:68:A:GLN:H   | 11       | 0.1           |
| (1,897) | 1:64:A:ASP:H   | 1:68:A:GLN:H   | 13       | 0.1           |
| (1,892) | 1:63:A:SER:HA  | 1:67:A:LYS:HG2 | 5        | 0.1           |
| (1,892) | 1:63:A:SER:HA  | 1:67:A:LYS:HG2 | 19       | 0.1           |
| (1,891) | 1:63:A:SER:H   | 1:65:A:GLU:H   | 6        | 0.1           |
| (1,886) | 1:62:A:GLU:HA  | 1:67:A:LYS:HG2 | 20       | 0.1           |
| (1,859) | 1:60:A:ASN:HB2 | 1:63:A:SER:HA  | 6        | 0.1           |
| (1,858) | 1:60:A:ASN:HA  | 1:66:A:THR:H   | 10       | 0.1           |
| (1,858) | 1:60:A:ASN:HA  | 1:66:A:THR:H   | 11       | 0.1           |
| (1,858) | 1:60:A:ASN:HA  | 1:66:A:THR:H   | 14       | 0.1           |
| (1,857) | 1:60:A:ASN:HB2 | 1:66:A:THR:HA  | 11       | 0.1           |
| (1,800) | 1:55:A:TYR:HB3 | 1:80:A:VAL:HA  | 9        | 0.1           |
| (1,800) | 1:55:A:TYR:HB3 | 1:80:A:VAL:HA  | 15       | 0.1           |
| (1,796) | 1:55:A:TYR:HB2 | 1:83:A:GLN:HB3 | 2        | 0.1           |
| (1,796) | 1:55:A:TYR:HB2 | 1:83:A:GLN:HB3 | 3        | 0.1           |
| (1,796) | 1:55:A:TYR:HB2 | 1:83:A:GLN:HB3 | 11       | 0.1           |
| (1,796) | 1:55:A:TYR:HB2 | 1:83:A:GLN:HB3 | 19       | 0.1           |
| (1,794) | 1:55:A:TYR:HB2 | 1:84:A:GLN:HG2 | 9        | 0.1           |
| (1,789) | 1:54:A:ARG:H   | 1:55:A:TYR:HA  | 8        | 0.1           |
| (1,789) | 1:54:A:ARG:H   | 1:55:A:TYR:HA  | 15       | 0.1           |
| (1,784) | 1:53:A:LYS:HA  | 1:55:A:TYR:H   | 6        | 0.1           |
| (1,741) | 1:51:A:LEU:H   | 1:52:A:LYS:HA  | 10       | 0.1           |
| (1,741) | 1:51:A:LEU:H   | 1:52:A:LYS:HA  | 14       | 0.1           |
| (1,740) | 1:51:A:LEU:H   | 1:52:A:LYS:HB3 | 10       | 0.1           |
| (1,724) | 1:50:A:ALA:H   | 1:52:A:LYS:HB3 | 20       | 0.1           |
| (1,723) | 1:50:A:ALA:H   | 1:51:A:LEU:HA  | 1        | 0.1           |
| (1,723) | 1:50:A:ALA:H   | 1:51:A:LEU:HA  | 9        | 0.1           |
| (1,722) | 1:50:A:ALA:HA  | 1:52:A:LYS:HB3 | 2        | 0.1           |
| (1,722) | 1:50:A:ALA:HA  | 1:52:A:LYS:HB3 | 8        | 0.1           |
| (1,722) | 1:50:A:ALA:HA  | 1:52:A:LYS:HB3 | 17       | 0.1           |
| (1,722) | 1:50:A:ALA:HA  | 1:52:A:LYS:HB3 | 20       | 0.1           |
| (1,709) | 1:49:A:LEU:HA  | 1:59:A:LEU:HG  | 12       | 0.1           |
| (1,707) | 1:49:A:LEU:HA  | 1:53:A:LYS:H   | 15       | 0.1           |
| (1,707) | 1:49:A:LEU:HA  | 1:53:A:LYS:H   | 20       | 0.1           |
| (1,706) | 1:48:A:GLY:H   | 1:50:A:ALA:H   | 10       | 0.1           |
| (1,692) | 1:48:A:GLY:HA2 | 1:51:A:LEU:HA  | 11       | 0.1           |
| (1,692) | 1:48:A:GLY:HA2 | 1:51:A:LEU:HA  | 17       | 0.1           |
| (1,692) | 1:48:A:GLY:HA2 | 1:51:A:LEU:HA  | 18       | 0.1           |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,691) | 1:48:A:GLY:HA3 | 1:51:A:LEU:HB3 | 1        | 0.1           |
| (1,691) | 1:48:A:GLY:HA3 | 1:51:A:LEU:HB3 | 3        | 0.1           |
| (1,691) | 1:48:A:GLY:HA3 | 1:51:A:LEU:HB3 | 4        | 0.1           |
| (1,691) | 1:48:A:GLY:HA3 | 1:51:A:LEU:HB3 | 5        | 0.1           |
| (1,691) | 1:48:A:GLY:HA3 | 1:51:A:LEU:HB3 | 12       | 0.1           |
| (1,691) | 1:48:A:GLY:HA3 | 1:51:A:LEU:HB3 | 16       | 0.1           |
| (1,691) | 1:48:A:GLY:HA3 | 1:51:A:LEU:HB3 | 17       | 0.1           |
| (1,688) | 1:48:A:GLY:HA2 | 1:59:A:LEU:HB3 | 2        | 0.1           |
| (1,688) | 1:48:A:GLY:HA2 | 1:59:A:LEU:HB3 | 11       | 0.1           |
| (1,688) | 1:48:A:GLY:HA2 | 1:59:A:LEU:HB3 | 14       | 0.1           |
| (1,687) | 1:48:A:GLY:HA2 | 1:59:A:LEU:HB2 | 5        | 0.1           |
| (1,687) | 1:48:A:GLY:HA2 | 1:59:A:LEU:HB2 | 8        | 0.1           |
| (1,687) | 1:48:A:GLY:HA2 | 1:59:A:LEU:HB2 | 18       | 0.1           |
| (1,676) | 1:47:A:LEU:HA  | 1:49:A:LEU:H   | 3        | 0.1           |
| (1,676) | 1:47:A:LEU:HA  | 1:49:A:LEU:H   | 11       | 0.1           |
| (1,676) | 1:47:A:LEU:HA  | 1:49:A:LEU:H   | 12       | 0.1           |
| (1,676) | 1:47:A:LEU:HA  | 1:49:A:LEU:H   | 17       | 0.1           |
| (1,675) | 1:47:A:LEU:HA  | 1:51:A:LEU:HA  | 8        | 0.1           |
| (1,675) | 1:47:A:LEU:HA  | 1:51:A:LEU:HA  | 16       | 0.1           |
| (1,674) | 1:47:A:LEU:HG  | 1:51:A:LEU:HB3 | 3        | 0.1           |
| (1,674) | 1:47:A:LEU:HG  | 1:51:A:LEU:HB3 | 7        | 0.1           |
| (1,674) | 1:47:A:LEU:HG  | 1:51:A:LEU:HB3 | 8        | 0.1           |
| (1,674) | 1:47:A:LEU:HG  | 1:51:A:LEU:HB3 | 16       | 0.1           |
| (1,673) | 1:47:A:LEU:HB3 | 1:51:A:LEU:HG  | 8        | 0.1           |
| (1,673) | 1:47:A:LEU:HB3 | 1:51:A:LEU:HG  | 20       | 0.1           |
| (1,665) | 1:46:A:GLU:H   | 1:47:A:LEU:HB2 | 3        | 0.1           |
| (1,665) | 1:46:A:GLU:H   | 1:47:A:LEU:HB2 | 5        | 0.1           |
| (1,665) | 1:46:A:GLU:H   | 1:47:A:LEU:HB2 | 20       | 0.1           |
| (1,651) | 1:45:A:LEU:HA  | 1:48:A:GLY:HA2 | 14       | 0.1           |
| (1,647) | 1:45:A:LEU:HA  | 1:49:A:LEU:HA  | 6        | 0.1           |
| (1,647) | 1:45:A:LEU:HA  | 1:49:A:LEU:HA  | 12       | 0.1           |
| (1,631) | 1:44:A:ALA:HA  | 1:47:A:LEU:HG  | 2        | 0.1           |
| (1,631) | 1:44:A:ALA:HA  | 1:47:A:LEU:HG  | 8        | 0.1           |
| (1,631) | 1:44:A:ALA:HA  | 1:47:A:LEU:HG  | 14       | 0.1           |
| (1,629) | 1:44:A:ALA:H   | 1:47:A:LEU:HB2 | 3        | 0.1           |
| (1,629) | 1:44:A:ALA:H   | 1:47:A:LEU:HB2 | 5        | 0.1           |
| (1,629) | 1:44:A:ALA:H   | 1:47:A:LEU:HB2 | 8        | 0.1           |
| (1,628) | 1:44:A:ALA:HA  | 1:48:A:GLY:HA3 | 4        | 0.1           |
| (1,618) | 1:43:A:ASP:HB3 | 1:46:A:GLU:H   | 7        | 0.1           |
| (1,618) | 1:43:A:ASP:HB3 | 1:46:A:GLU:H   | 8        | 0.1           |
| (1,618) | 1:43:A:ASP:HB3 | 1:46:A:GLU:H   | 9        | 0.1           |
| (1,616) | 1:43:A:ASP:HA  | 1:46:A:GLU:HA  | 1        | 0.1           |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,616) | 1:43:A:ASP:HA   | 1:46:A:GLU:HA  | 3        | 0.1           |
| (1,601) | 1:41:A:SER:HA   | 1:44:A:ALA:HA  | 4        | 0.1           |
| (1,601) | 1:41:A:SER:HA   | 1:44:A:ALA:HA  | 7        | 0.1           |
| (1,572) | 1:39:A:LEU:HA   | 1:43:A:ASP:H   | 5        | 0.1           |
| (1,545) | 1:33:A:PHE:HE1  | 1:40:A:ASP:H   | 6        | 0.1           |
| (1,535) | 1:33:A:PHE:HA   | 1:39:A:LEU:HB3 | 3        | 0.1           |
| (1,517) | 1:32:A:LEU:HB2  | 1:39:A:LEU:H   | 18       | 0.1           |
| (1,503) | 1:31:A:PRO:HB2  | 1:35:A:GLU:HB3 | 9        | 0.1           |
| (1,480) | 1:29:A:GLU:H    | 1:74:A:GLN:HB3 | 13       | 0.1           |
| (1,480) | 1:29:A:GLU:H    | 1:74:A:GLN:HB3 | 14       | 0.1           |
| (1,479) | 1:29:A:GLU:HA   | 1:72:A:SER:H   | 6        | 0.1           |
| (1,479) | 1:29:A:GLU:HA   | 1:72:A:SER:H   | 16       | 0.1           |
| (1,414) | 1:21:A:ILE:HG13 | 1:25:A:ASP:HB2 | 4        | 0.1           |
| (1,414) | 1:21:A:ILE:HG13 | 1:25:A:ASP:HB2 | 7        | 0.1           |
| (1,406) | 1:19:A:GLU:HB3  | 1:21:A:ILE:H   | 11       | 0.1           |
| (1,388) | 1:18:A:LEU:HB3  | 1:21:A:ILE:HA  | 1        | 0.1           |
| (1,388) | 1:18:A:LEU:HB3  | 1:21:A:ILE:HA  | 8        | 0.1           |
| (1,388) | 1:18:A:LEU:HB3  | 1:21:A:ILE:HA  | 9        | 0.1           |
| (1,388) | 1:18:A:LEU:HB3  | 1:21:A:ILE:HA  | 18       | 0.1           |
| (1,362) | 1:16:A:LEU:HG   | 1:43:A:ASP:HB2 | 11       | 0.1           |
| (1,357) | 1:16:A:LEU:HB2  | 1:18:A:LEU:HA  | 1        | 0.1           |
| (1,357) | 1:16:A:LEU:HB2  | 1:18:A:LEU:HA  | 4        | 0.1           |
| (1,337) | 1:15:A:VAL:HB   | 1:51:A:LEU:HG  | 15       | 0.1           |
| (1,289) | 1:12:A:ILE:HG13 | 1:15:A:VAL:H   | 1        | 0.1           |
| (1,289) | 1:12:A:ILE:HG13 | 1:15:A:VAL:H   | 6        | 0.1           |
| (1,289) | 1:12:A:ILE:HG13 | 1:15:A:VAL:H   | 9        | 0.1           |
| (1,289) | 1:12:A:ILE:HG13 | 1:15:A:VAL:H   | 10       | 0.1           |
| (1,289) | 1:12:A:ILE:HG13 | 1:15:A:VAL:H   | 13       | 0.1           |
| (1,289) | 1:12:A:ILE:HG13 | 1:15:A:VAL:H   | 17       | 0.1           |
| (1,289) | 1:12:A:ILE:HG13 | 1:15:A:VAL:H   | 20       | 0.1           |
| (1,286) | 1:12:A:ILE:H    | 1:14:A:ASP:H   | 8        | 0.1           |
| (1,286) | 1:12:A:ILE:H    | 1:14:A:ASP:H   | 13       | 0.1           |
| (1,286) | 1:12:A:ILE:H    | 1:14:A:ASP:H   | 15       | 0.1           |
| (1,286) | 1:12:A:ILE:H    | 1:14:A:ASP:H   | 17       | 0.1           |
| (1,286) | 1:12:A:ILE:H    | 1:14:A:ASP:H   | 18       | 0.1           |
| (1,263) | 1:11:A:MET:HB3  | 1:15:A:VAL:H   | 12       | 0.1           |
| (1,258) | 1:11:A:MET:HB2  | 1:15:A:VAL:HB  | 3        | 0.1           |
| (1,258) | 1:11:A:MET:HB2  | 1:15:A:VAL:HB  | 12       | 0.1           |
| (1,257) | 1:11:A:MET:HA   | 1:15:A:VAL:HA  | 10       | 0.1           |
| (1,257) | 1:11:A:MET:HA   | 1:15:A:VAL:HA  | 12       | 0.1           |
| (1,257) | 1:11:A:MET:HA   | 1:15:A:VAL:HA  | 13       | 0.1           |
| (1,257) | 1:11:A:MET:HA   | 1:15:A:VAL:HA  | 20       | 0.1           |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,232) | 1:10:A:GLN:HG3 | 1:23:A:ILE:HG13 | 9        | 0.1           |
| (1,232) | 1:10:A:GLN:HG3 | 1:23:A:ILE:HG13 | 17       | 0.1           |
| (1,231) | 1:10:A:GLN:HA  | 1:12:A:ILE:HB   | 5        | 0.1           |
| (1,231) | 1:10:A:GLN:HA  | 1:12:A:ILE:HB   | 9        | 0.1           |
| (1,230) | 1:10:A:GLN:HB2 | 1:14:A:ASP:H    | 2        | 0.1           |
| (1,230) | 1:10:A:GLN:HB2 | 1:14:A:ASP:H    | 5        | 0.1           |
| (1,230) | 1:10:A:GLN:HB2 | 1:14:A:ASP:H    | 11       | 0.1           |
| (1,230) | 1:10:A:GLN:HB2 | 1:14:A:ASP:H    | 15       | 0.1           |
| (1,230) | 1:10:A:GLN:HB2 | 1:14:A:ASP:H    | 16       | 0.1           |
| (1,230) | 1:10:A:GLN:HB2 | 1:14:A:ASP:H    | 19       | 0.1           |
| (1,230) | 1:10:A:GLN:HB2 | 1:14:A:ASP:H    | 20       | 0.1           |
| (1,229) | 1:10:A:GLN:H   | 1:14:A:ASP:HB3  | 5        | 0.1           |
| (1,229) | 1:10:A:GLN:H   | 1:14:A:ASP:HB3  | 10       | 0.1           |
| (1,229) | 1:10:A:GLN:H   | 1:14:A:ASP:HB3  | 11       | 0.1           |
| (1,229) | 1:10:A:GLN:H   | 1:14:A:ASP:HB3  | 16       | 0.1           |
| (1,229) | 1:10:A:GLN:H   | 1:14:A:ASP:HB3  | 18       | 0.1           |
| (1,229) | 1:10:A:GLN:H   | 1:14:A:ASP:HB3  | 19       | 0.1           |
| (1,228) | 1:10:A:GLN:HG3 | 1:22:A:THR:HA   | 2        | 0.1           |
| (1,228) | 1:10:A:GLN:HG3 | 1:22:A:THR:HA   | 3        | 0.1           |
| (1,228) | 1:10:A:GLN:HG3 | 1:22:A:THR:HA   | 4        | 0.1           |
| (1,228) | 1:10:A:GLN:HG3 | 1:22:A:THR:HA   | 9        | 0.1           |
| (1,228) | 1:10:A:GLN:HG3 | 1:22:A:THR:HA   | 10       | 0.1           |
| (1,228) | 1:10:A:GLN:HG3 | 1:22:A:THR:HA   | 15       | 0.1           |
| (1,227) | 1:10:A:GLN:HG2 | 1:14:A:ASP:HA   | 3        | 0.1           |
| (1,226) | 1:10:A:GLN:HB3 | 1:14:A:ASP:H    | 2        | 0.1           |
| (1,226) | 1:10:A:GLN:HB3 | 1:14:A:ASP:H    | 7        | 0.1           |
| (1,226) | 1:10:A:GLN:HB3 | 1:14:A:ASP:H    | 8        | 0.1           |
| (1,226) | 1:10:A:GLN:HB3 | 1:14:A:ASP:H    | 11       | 0.1           |
| (1,226) | 1:10:A:GLN:HB3 | 1:14:A:ASP:H    | 12       | 0.1           |
| (1,226) | 1:10:A:GLN:HB3 | 1:14:A:ASP:H    | 13       | 0.1           |
| (1,226) | 1:10:A:GLN:HB3 | 1:14:A:ASP:H    | 14       | 0.1           |
| (1,226) | 1:10:A:GLN:HB3 | 1:14:A:ASP:H    | 16       | 0.1           |
| (1,226) | 1:10:A:GLN:HB3 | 1:14:A:ASP:H    | 17       | 0.1           |
| (1,226) | 1:10:A:GLN:HB3 | 1:14:A:ASP:H    | 18       | 0.1           |
| (1,225) | 1:10:A:GLN:HA  | 1:13:A:ILE:HA   | 1        | 0.1           |
| (1,225) | 1:10:A:GLN:HA  | 1:13:A:ILE:HA   | 4        | 0.1           |
| (1,225) | 1:10:A:GLN:HA  | 1:13:A:ILE:HA   | 19       | 0.1           |
| (1,225) | 1:10:A:GLN:HA  | 1:13:A:ILE:HA   | 20       | 0.1           |
| (1,224) | 1:10:A:GLN:H   | 1:12:A:ILE:HA   | 2        | 0.1           |
| (1,224) | 1:10:A:GLN:H   | 1:12:A:ILE:HA   | 4        | 0.1           |
| (1,224) | 1:10:A:GLN:H   | 1:12:A:ILE:HA   | 5        | 0.1           |
| (1,224) | 1:10:A:GLN:H   | 1:12:A:ILE:HA   | 8        | 0.1           |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,224) | 1:10:A:GLN:H   | 1:12:A:ILE:HA   | 10       | 0.1           |
| (1,224) | 1:10:A:GLN:H   | 1:12:A:ILE:HA   | 11       | 0.1           |
| (1,224) | 1:10:A:GLN:H   | 1:12:A:ILE:HA   | 13       | 0.1           |
| (1,224) | 1:10:A:GLN:H   | 1:12:A:ILE:HA   | 16       | 0.1           |
| (1,224) | 1:10:A:GLN:H   | 1:12:A:ILE:HA   | 17       | 0.1           |
| (1,224) | 1:10:A:GLN:H   | 1:12:A:ILE:HA   | 19       | 0.1           |
| (1,223) | 1:10:A:GLN:HB2 | 1:22:A:THR:HB   | 2        | 0.1           |
| (1,223) | 1:10:A:GLN:HB2 | 1:22:A:THR:HB   | 9        | 0.1           |
| (1,223) | 1:10:A:GLN:HB2 | 1:22:A:THR:HB   | 20       | 0.1           |
| (1,191) | 1:9:A:LYS:HA   | 1:13:A:ILE:HA   | 10       | 0.1           |
| (1,191) | 1:9:A:LYS:HA   | 1:13:A:ILE:HA   | 15       | 0.1           |
| (1,191) | 1:9:A:LYS:HA   | 1:13:A:ILE:HA   | 16       | 0.1           |
| (1,190) | 1:9:A:LYS:HA   | 1:73:A:ILE:HB   | 6        | 0.1           |
| (1,190) | 1:9:A:LYS:HA   | 1:73:A:ILE:HB   | 10       | 0.1           |
| (1,190) | 1:9:A:LYS:HA   | 1:73:A:ILE:HB   | 14       | 0.1           |
| (1,187) | 1:9:A:LYS:H    | 1:12:A:ILE:HB   | 3        | 0.1           |
| (1,187) | 1:9:A:LYS:H    | 1:12:A:ILE:HB   | 5        | 0.1           |
| (1,187) | 1:9:A:LYS:H    | 1:12:A:ILE:HB   | 8        | 0.1           |
| (1,187) | 1:9:A:LYS:H    | 1:12:A:ILE:HB   | 13       | 0.1           |
| (1,187) | 1:9:A:LYS:H    | 1:12:A:ILE:HB   | 15       | 0.1           |
| (1,187) | 1:9:A:LYS:H    | 1:12:A:ILE:HB   | 17       | 0.1           |
| (1,187) | 1:9:A:LYS:H    | 1:12:A:ILE:HB   | 20       | 0.1           |
| (1,186) | 1:9:A:LYS:H    | 1:11:A:MET:HB2  | 8        | 0.1           |
| (1,186) | 1:9:A:LYS:H    | 1:11:A:MET:HB2  | 9        | 0.1           |
| (1,186) | 1:9:A:LYS:H    | 1:11:A:MET:HB2  | 13       | 0.1           |
| (1,186) | 1:9:A:LYS:H    | 1:11:A:MET:HB2  | 17       | 0.1           |
| (1,185) | 1:9:A:LYS:HB3  | 1:12:A:ILE:H    | 8        | 0.1           |
| (1,185) | 1:9:A:LYS:HB3  | 1:12:A:ILE:H    | 11       | 0.1           |
| (1,185) | 1:9:A:LYS:HB3  | 1:12:A:ILE:H    | 13       | 0.1           |
| (1,185) | 1:9:A:LYS:HB3  | 1:12:A:ILE:H    | 17       | 0.1           |
| (1,184) | 1:9:A:LYS:HB2  | 1:13:A:ILE:HG13 | 3        | 0.1           |
| (1,184) | 1:9:A:LYS:HB2  | 1:13:A:ILE:HG13 | 8        | 0.1           |
| (1,184) | 1:9:A:LYS:HB2  | 1:13:A:ILE:HG13 | 10       | 0.1           |
| (1,184) | 1:9:A:LYS:HB2  | 1:13:A:ILE:HG13 | 16       | 0.1           |
| (1,184) | 1:9:A:LYS:HB2  | 1:13:A:ILE:HG13 | 20       | 0.1           |
| (1,183) | 1:9:A:LYS:HB2  | 1:13:A:ILE:H    | 9        | 0.1           |
| (1,183) | 1:9:A:LYS:HB2  | 1:13:A:ILE:H    | 19       | 0.1           |
| (1,182) | 1:9:A:LYS:HA   | 1:13:A:ILE:HB   | 16       | 0.1           |
| (1,143) | 1:8:A:LEU:HA   | 1:12:A:ILE:HA   | 3        | 0.1           |
| (1,143) | 1:8:A:LEU:HA   | 1:12:A:ILE:HA   | 12       | 0.1           |
| (1,143) | 1:8:A:LEU:HA   | 1:12:A:ILE:HA   | 14       | 0.1           |
| (1,143) | 1:8:A:LEU:HA   | 1:12:A:ILE:HA   | 17       | 0.1           |

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| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,143) | 1:8:A:LEU:HA  | 1:12:A:ILE:HA   | 20       | 0.1           |
| (1,142) | 1:8:A:LEU:HA  | 1:11:A:MET:HA   | 11       | 0.1           |
| (1,142) | 1:8:A:LEU:HA  | 1:11:A:MET:HA   | 13       | 0.1           |
| (1,142) | 1:8:A:LEU:HA  | 1:11:A:MET:HA   | 19       | 0.1           |
| (1,138) | 1:8:A:LEU:HB2 | 1:11:A:MET:H    | 6        | 0.1           |
| (1,138) | 1:8:A:LEU:HB2 | 1:11:A:MET:H    | 11       | 0.1           |
| (1,138) | 1:8:A:LEU:HB2 | 1:11:A:MET:H    | 13       | 0.1           |
| (1,138) | 1:8:A:LEU:HB2 | 1:11:A:MET:H    | 14       | 0.1           |
| (1,138) | 1:8:A:LEU:HB2 | 1:11:A:MET:H    | 15       | 0.1           |
| (1,138) | 1:8:A:LEU:HB2 | 1:11:A:MET:H    | 17       | 0.1           |
| (1,137) | 1:8:A:LEU:HA  | 1:76:A:LEU:HB2  | 9        | 0.1           |
| (1,137) | 1:8:A:LEU:HA  | 1:76:A:LEU:HB2  | 10       | 0.1           |
| (1,137) | 1:8:A:LEU:HA  | 1:76:A:LEU:HB2  | 17       | 0.1           |
| (1,136) | 1:8:A:LEU:HB3 | 1:12:A:ILE:HA   | 2        | 0.1           |
| (1,136) | 1:8:A:LEU:HB3 | 1:12:A:ILE:HA   | 10       | 0.1           |
| (1,133) | 1:8:A:LEU:HB2 | 1:12:A:ILE:HG13 | 1        | 0.1           |
| (1,133) | 1:8:A:LEU:HB2 | 1:12:A:ILE:HG13 | 2        | 0.1           |
| (1,133) | 1:8:A:LEU:HB2 | 1:12:A:ILE:HG13 | 6        | 0.1           |
| (1,133) | 1:8:A:LEU:HB2 | 1:12:A:ILE:HG13 | 8        | 0.1           |
| (1,133) | 1:8:A:LEU:HB2 | 1:12:A:ILE:HG13 | 10       | 0.1           |
| (1,133) | 1:8:A:LEU:HB2 | 1:12:A:ILE:HG13 | 14       | 0.1           |
| (1,133) | 1:8:A:LEU:HB2 | 1:12:A:ILE:HG13 | 18       | 0.1           |
| (1,131) | 1:8:A:LEU:HA  | 1:12:A:ILE:HG12 | 5        | 0.1           |
| (1,131) | 1:8:A:LEU:HA  | 1:12:A:ILE:HG12 | 8        | 0.1           |
| (1,127) | 1:8:A:LEU:HA  | 1:12:A:ILE:HB   | 3        | 0.1           |
| (1,127) | 1:8:A:LEU:HA  | 1:12:A:ILE:HB   | 5        | 0.1           |
| (1,127) | 1:8:A:LEU:HA  | 1:12:A:ILE:HB   | 9        | 0.1           |
| (1,127) | 1:8:A:LEU:HA  | 1:12:A:ILE:HB   | 10       | 0.1           |
| (1,127) | 1:8:A:LEU:HA  | 1:12:A:ILE:HB   | 17       | 0.1           |
| (1,113) | 1:7:A:GLU:HA  | 1:11:A:MET:HB3  | 13       | 0.1           |
| (1,113) | 1:7:A:GLU:HA  | 1:11:A:MET:HB3  | 20       | 0.1           |
| (1,111) | 1:7:A:GLU:H   | 1:10:A:GLN:HB2  | 5        | 0.1           |
| (1,111) | 1:7:A:GLU:H   | 1:10:A:GLN:HB2  | 9        | 0.1           |
| (1,111) | 1:7:A:GLU:H   | 1:10:A:GLN:HB2  | 13       | 0.1           |
| (1,111) | 1:7:A:GLU:H   | 1:10:A:GLN:HB2  | 16       | 0.1           |
| (1,111) | 1:7:A:GLU:H   | 1:10:A:GLN:HB2  | 17       | 0.1           |
| (1,95)  | 1:6:A:ASP:HB2 | 1:8:A:LEU:H     | 2        | 0.1           |
| (1,95)  | 1:6:A:ASP:HB2 | 1:8:A:LEU:H     | 3        | 0.1           |
| (1,95)  | 1:6:A:ASP:HB2 | 1:8:A:LEU:H     | 15       | 0.1           |
| (1,68)  | 1:5:A:ALA:HA  | 1:9:A:LYS:HB2   | 6        | 0.1           |
| (1,68)  | 1:5:A:ALA:HA  | 1:9:A:LYS:HB2   | 11       | 0.1           |
| (1,68)  | 1:5:A:ALA:HA  | 1:9:A:LYS:HB2   | 17       | 0.1           |

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| Key    | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|--------|---------------|-----------------|----------|---------------|
| (1,27) | 1:4:A:LEU:HB2 | 1:84:A:GLN:HG3  | 18       | 0.1           |
| (1,26) | 1:4:A:LEU:HB3 | 1:81:A:GLU:HA   | 16       | 0.1           |
| (1,23) | 1:4:A:LEU:HA  | 1:8:A:LEU:HB2   | 6        | 0.1           |
| (1,23) | 1:4:A:LEU:HA  | 1:8:A:LEU:HB2   | 9        | 0.1           |
| (1,23) | 1:4:A:LEU:HA  | 1:8:A:LEU:HB2   | 11       | 0.1           |
| (1,23) | 1:4:A:LEU:HA  | 1:8:A:LEU:HB2   | 13       | 0.1           |
| (1,23) | 1:4:A:LEU:HA  | 1:8:A:LEU:HB2   | 14       | 0.1           |
| (1,23) | 1:4:A:LEU:HA  | 1:8:A:LEU:HB2   | 16       | 0.1           |
| (1,22) | 1:4:A:LEU:HB2 | 1:77:A:VAL:HA   | 6        | 0.1           |
| (1,22) | 1:4:A:LEU:HB2 | 1:77:A:VAL:HA   | 11       | 0.1           |
| (1,22) | 1:4:A:LEU:HB2 | 1:77:A:VAL:HA   | 13       | 0.1           |
| (1,19) | 1:4:A:LEU:HG  | 1:81:A:GLU:HA   | 12       | 0.1           |
| (1,18) | 1:4:A:LEU:HA  | 1:8:A:LEU:HA    | 2        | 0.1           |
| (1,18) | 1:4:A:LEU:HA  | 1:8:A:LEU:HA    | 10       | 0.1           |
| (1,18) | 1:4:A:LEU:HA  | 1:8:A:LEU:HA    | 15       | 0.1           |
| (1,16) | 1:4:A:LEU:HB2 | 1:77:A:VAL:HB   | 9        | 0.1           |
| (1,15) | 1:4:A:LEU:HG  | 1:7:A:GLU:HB2   | 18       | 0.1           |
| (1,14) | 1:4:A:LEU:HB2 | 1:8:A:LEU:HB2   | 8        | 0.1           |
| (1,14) | 1:4:A:LEU:HB2 | 1:8:A:LEU:HB2   | 18       | 0.1           |
| (1,13) | 1:4:A:LEU:HG  | 1:8:A:LEU:HA    | 8        | 0.1           |
| (1,12) | 1:4:A:LEU:HA  | 1:7:A:GLU:HA    | 12       | 0.1           |
| (1,7)  | 1:3:A:ASN:H   | 1:84:A:GLN:HE22 | 13       | 0.1           |
| (1,2)  | 1:2:A:SER:H   | 1:4:A:LEU:HB3   | 9        | 0.1           |

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

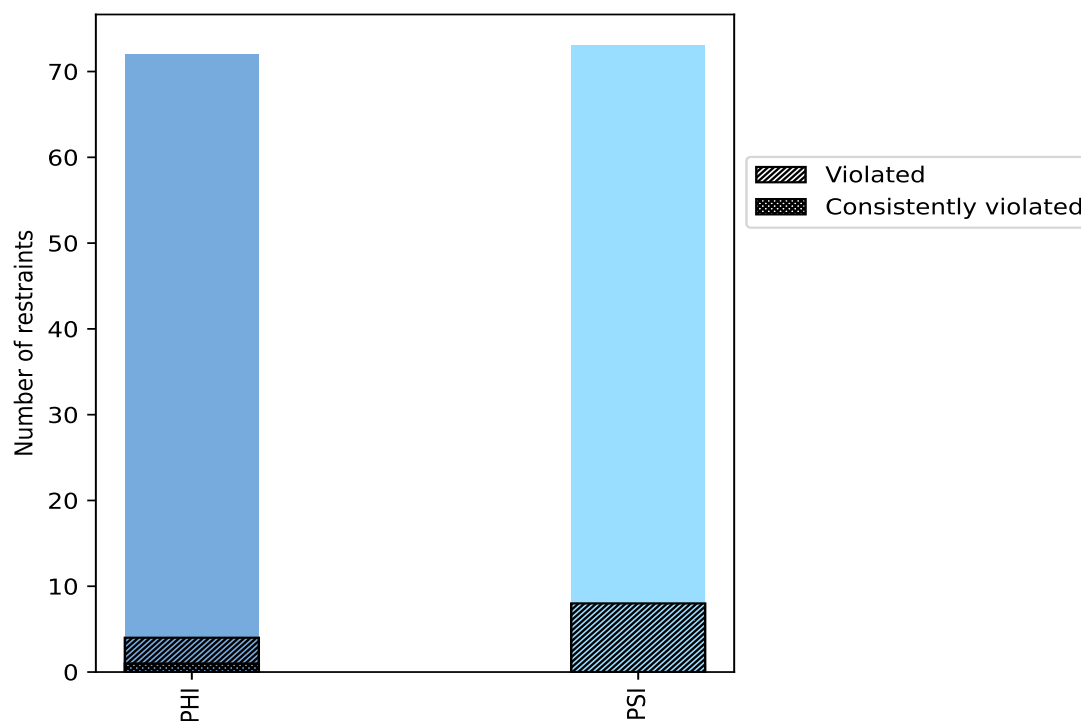
### 10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PHI        | 72    | 49.7           | 4                     | 5.6            | 2.8            | 1                                  | 1.4            | 0.7            |
| PSI        | 73    | 50.3           | 8                     | 11.0           | 5.5            | 0                                  | 0.0            | 0.0            |
| Total      | 145   | 100.0          | 12                    | 8.3            | 8.3            | 1                                  | 0.7            | 0.7            |

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

#### 10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



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

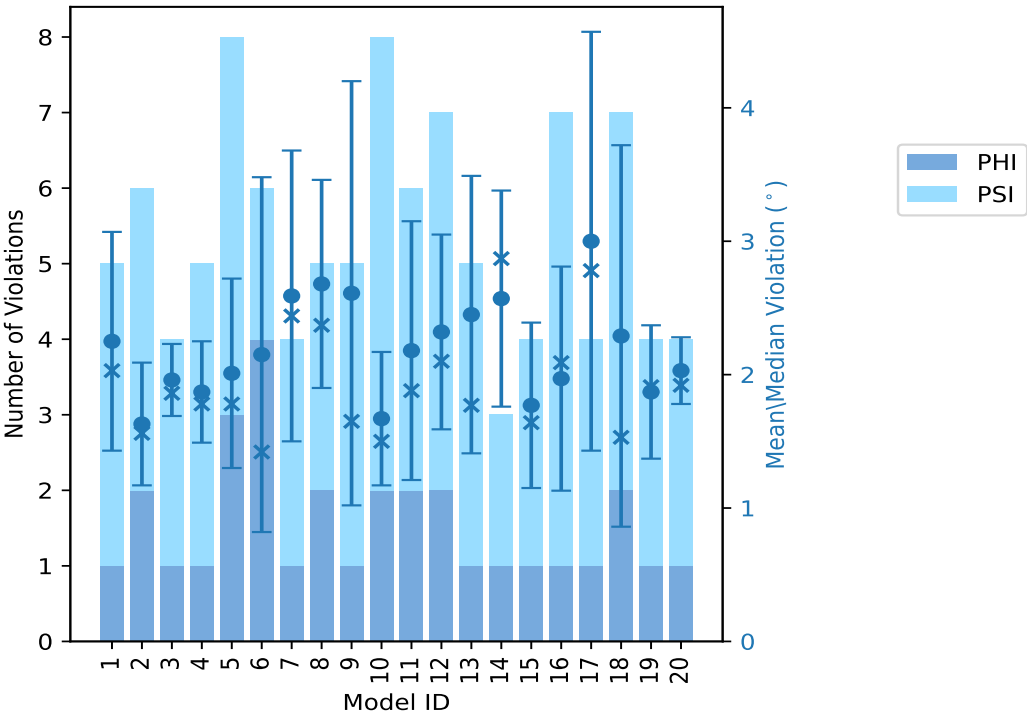


## 10.2 Dihedral-angle violation statistics for each model

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PHI                  | PSI | Total |          |         |        |            |
| 1        | 1                    | 4   | 5     | 2.25     | 3.37    | 0.82   | 2.03       |
| 2        | 2                    | 4   | 6     | 1.63     | 2.37    | 0.46   | 1.56       |
| 3        | 1                    | 3   | 4     | 1.96     | 2.38    | 0.27   | 1.86       |
| 4        | 1                    | 4   | 5     | 1.87     | 2.44    | 0.38   | 1.78       |
| 5        | 3                    | 5   | 8     | 2.01     | 3.45    | 0.71   | 1.78       |
| 6        | 4                    | 2   | 6     | 2.15     | 4.58    | 1.33   | 1.42       |
| 7        | 1                    | 3   | 4     | 2.59     | 3.98    | 1.09   | 2.44       |
| 8        | 2                    | 3   | 5     | 2.68     | 3.87    | 0.78   | 2.37       |
| 9        | 1                    | 4   | 5     | 2.61     | 5.06    | 1.59   | 1.65       |
| 10       | 2                    | 6   | 8     | 1.67     | 2.48    | 0.5    | 1.5        |
| 11       | 2                    | 4   | 6     | 2.18     | 3.82    | 0.97   | 1.88       |
| 12       | 2                    | 5   | 7     | 2.32     | 3.71    | 0.73   | 2.1        |
| 13       | 1                    | 4   | 5     | 2.45     | 4.02    | 1.04   | 1.77       |
| 14       | 1                    | 2   | 3     | 2.57     | 3.37    | 0.81   | 2.87       |
| 15       | 1                    | 3   | 4     | 1.77     | 2.76    | 0.62   | 1.64       |
| 16       | 1                    | 6   | 7     | 1.97     | 3.62    | 0.84   | 2.09       |
| 17       | 1                    | 3   | 4     | 3.0      | 5.01    | 1.57   | 2.78       |
| 18       | 2                    | 5   | 7     | 2.29     | 4.92    | 1.43   | 1.53       |
| 19       | 1                    | 3   | 4     | 1.87     | 2.51    | 0.5    | 1.91       |
| 20       | 1                    | 3   | 4     | 2.03     | 2.45    | 0.25   | 1.92       |

10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



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

10.3 Dihedral-angle violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

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

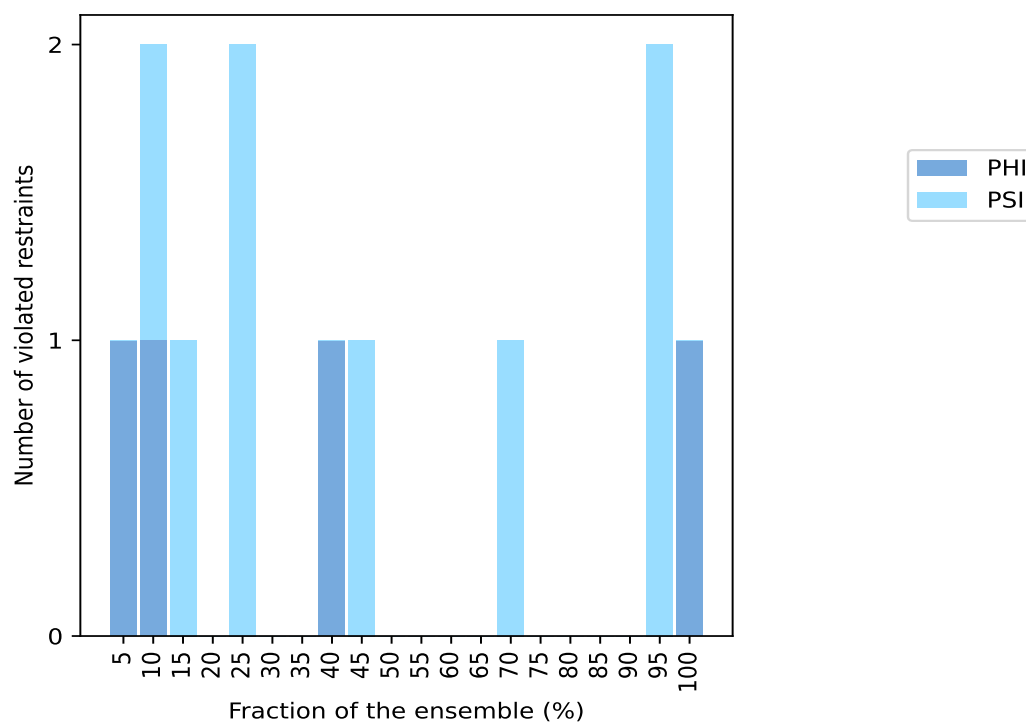
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PHI                           | PSI | Total | Count <sup>1</sup>       | %     |
| 0                             | 0   | 0     | 12                       | 60.0  |
| 0                             | 0   | 0     | 13                       | 65.0  |
| 0                             | 1   | 1     | 14                       | 70.0  |
| 0                             | 0   | 0     | 15                       | 75.0  |
| 0                             | 0   | 0     | 16                       | 80.0  |
| 0                             | 0   | 0     | 17                       | 85.0  |
| 0                             | 0   | 0     | 18                       | 90.0  |
| 0                             | 2   | 2     | 19                       | 95.0  |
| 1                             | 0   | 1     | 20                       | 100.0 |

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

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

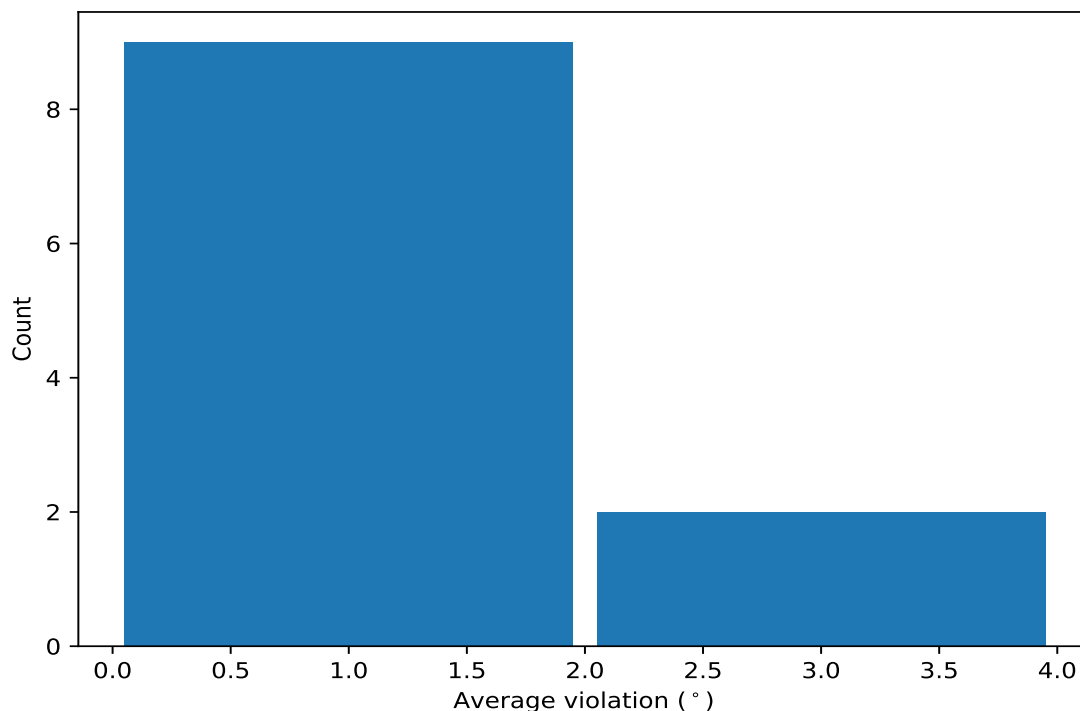


## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

### 10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

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

in the ensemble



#### 10.4.2 Table: Most violated dihedral-angle restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

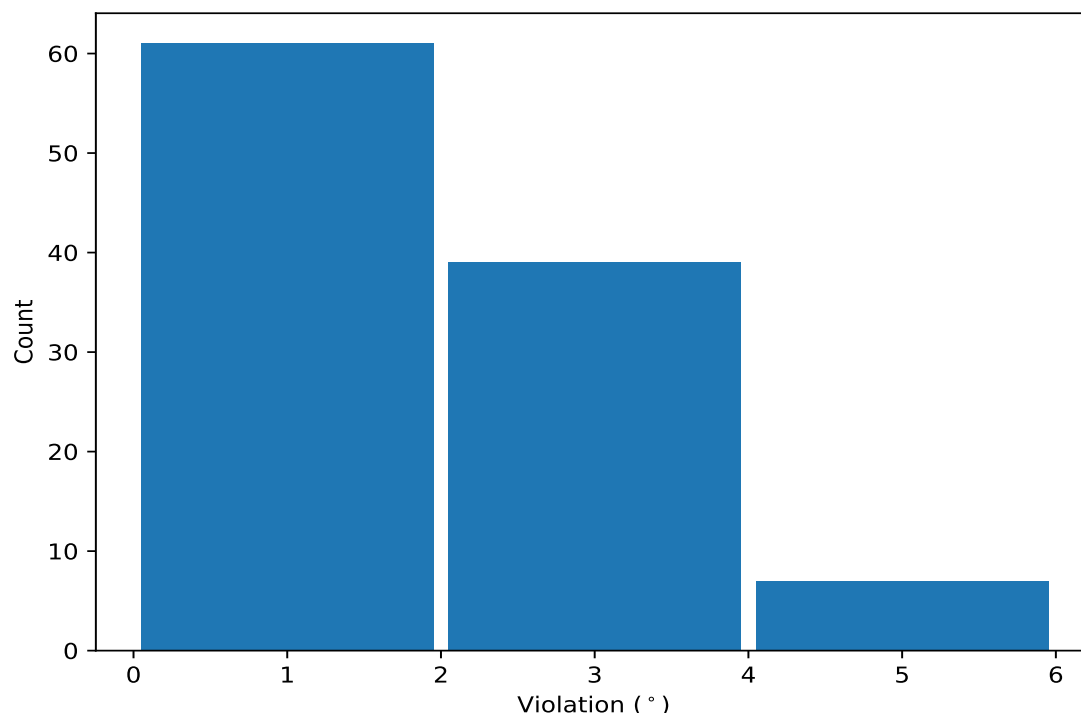
| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|--------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,41) | 1:25:A:ASP:C | 1:26:A:ILE:N  | 1:26:A:ILE:CA | 1:26:A:ILE:C | 20                  | 2.67 | 0.89            | 2.9    |
| (1,40) | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C  | 1:26:A:ILE:N | 19                  | 3.51 | 0.96            | 3.62   |
| (1,38) | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:ASP:N | 19                  | 1.75 | 0.3             | 1.8    |
| (1,91) | 1:58:A:HIS:N | 1:58:A:HIS:CA | 1:58:A:HIS:C  | 1:59:A:LEU:N | 14                  | 1.58 | 0.32            | 1.63   |
| (1,44) | 1:27:A:ASP:N | 1:27:A:ASP:CA | 1:27:A:ASP:C  | 1:28:A:THR:N | 9                   | 1.78 | 0.33            | 1.76   |
| (1,88) | 1:56:A:ASN:C | 1:57:A:ILE:N  | 1:57:A:ILE:CA | 1:57:A:ILE:C | 8                   | 1.86 | 0.54            | 2.1    |
| (1,46) | 1:28:A:THR:N | 1:28:A:THR:CA | 1:28:A:THR:C  | 1:29:A:GLU:N | 5                   | 1.77 | 0.6             | 1.56   |
| (1,97) | 1:61:A:ALA:N | 1:61:A:ALA:CA | 1:61:A:ALA:C  | 1:62:A:GLU:N | 5                   | 1.32 | 0.12            | 1.35   |
| (1,81) | 1:53:A:LYS:N | 1:53:A:LYS:CA | 1:53:A:LYS:C  | 1:54:A:ARG:N | 3                   | 1.24 | 0.03            | 1.25   |
| (1,94) | 1:59:A:LEU:C | 1:60:A:ASN:N  | 1:60:A:ASN:CA | 1:60:A:ASN:C | 2                   | 1.12 | 0.01            | 1.12   |
| (1,85) | 1:55:A:TYR:N | 1:55:A:TYR:CA | 1:55:A:TYR:C  | 1:56:A:ASN:N | 2                   | 1.06 | 0.01            | 1.06   |

<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 (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,40) | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C  | 1:26:A:ILE:N | 9        | 5.06          |
| (1,40) | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C  | 1:26:A:ILE:N | 17       | 5.01          |
| (1,40) | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C  | 1:26:A:ILE:N | 18       | 4.92          |
| (1,40) | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C  | 1:26:A:ILE:N | 6        | 4.58          |
| (1,41) | 1:25:A:ASP:C | 1:26:A:ILE:N  | 1:26:A:ILE:CA | 1:26:A:ILE:C | 17       | 4.07          |
| (1,41) | 1:25:A:ASP:C | 1:26:A:ILE:N  | 1:26:A:ILE:CA | 1:26:A:ILE:C | 18       | 4.05          |
| (1,40) | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C  | 1:26:A:ILE:N | 13       | 4.02          |
| (1,40) | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C  | 1:26:A:ILE:N | 7        | 3.98          |
| (1,41) | 1:25:A:ASP:C | 1:26:A:ILE:N  | 1:26:A:ILE:CA | 1:26:A:ILE:C | 9        | 3.94          |
| (1,40) | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C  | 1:26:A:ILE:N | 8        | 3.87          |
| (1,40) | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C  | 1:26:A:ILE:N | 11       | 3.82          |
| (1,40) | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C  | 1:26:A:ILE:N | 12       | 3.71          |
| (1,40) | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C  | 1:26:A:ILE:N | 16       | 3.62          |
| (1,40) | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C  | 1:26:A:ILE:N | 5        | 3.45          |

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| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,40) | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C  | 1:26:A:ILE:N | 1        | 3.37          |
| (1,40) | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C  | 1:26:A:ILE:N | 14       | 3.37          |
| (1,41) | 1:25:A:ASP:C | 1:26:A:ILE:N  | 1:26:A:ILE:CA | 1:26:A:ILE:C | 13       | 3.35          |
| (1,41) | 1:25:A:ASP:C | 1:26:A:ILE:N  | 1:26:A:ILE:CA | 1:26:A:ILE:C | 7        | 3.32          |
| (1,41) | 1:25:A:ASP:C | 1:26:A:ILE:N  | 1:26:A:ILE:CA | 1:26:A:ILE:C | 8        | 3.31          |
| (1,41) | 1:25:A:ASP:C | 1:26:A:ILE:N  | 1:26:A:ILE:CA | 1:26:A:ILE:C | 6        | 3.27          |
| (1,41) | 1:25:A:ASP:C | 1:26:A:ILE:N  | 1:26:A:ILE:CA | 1:26:A:ILE:C | 11       | 2.99          |
| (1,41) | 1:25:A:ASP:C | 1:26:A:ILE:N  | 1:26:A:ILE:CA | 1:26:A:ILE:C | 1        | 2.96          |
| (1,41) | 1:25:A:ASP:C | 1:26:A:ILE:N  | 1:26:A:ILE:CA | 1:26:A:ILE:C | 12       | 2.94          |
| (1,41) | 1:25:A:ASP:C | 1:26:A:ILE:N  | 1:26:A:ILE:CA | 1:26:A:ILE:C | 14       | 2.87          |
| (1,41) | 1:25:A:ASP:C | 1:26:A:ILE:N  | 1:26:A:ILE:CA | 1:26:A:ILE:C | 5        | 2.83          |
| (1,46) | 1:28:A:THR:N | 1:28:A:THR:CA | 1:28:A:THR:C  | 1:29:A:GLU:N | 15       | 2.76          |
| (1,40) | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C  | 1:26:A:ILE:N | 19       | 2.51          |
| (1,40) | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C  | 1:26:A:ILE:N | 10       | 2.48          |
| (1,40) | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C  | 1:26:A:ILE:N | 20       | 2.45          |
| (1,40) | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C  | 1:26:A:ILE:N | 4        | 2.44          |
| (1,44) | 1:27:A:ASP:N | 1:27:A:ASP:CA | 1:27:A:ASP:C  | 1:28:A:THR:N | 16       | 2.41          |
| (1,40) | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C  | 1:26:A:ILE:N | 3        | 2.38          |
| (1,88) | 1:56:A:ASN:C | 1:57:A:ILE:N  | 1:57:A:ILE:CA | 1:57:A:ILE:C | 2        | 2.37          |
| (1,88) | 1:56:A:ASN:C | 1:57:A:ILE:N  | 1:57:A:ILE:CA | 1:57:A:ILE:C | 8        | 2.37          |
| (1,88) | 1:56:A:ASN:C | 1:57:A:ILE:N  | 1:57:A:ILE:CA | 1:57:A:ILE:C | 12       | 2.34          |
| (1,88) | 1:56:A:ASN:C | 1:57:A:ILE:N  | 1:57:A:ILE:CA | 1:57:A:ILE:C | 11       | 2.33          |
| (1,91) | 1:58:A:HIS:N | 1:58:A:HIS:CA | 1:58:A:HIS:C  | 1:59:A:LEU:N | 10       | 2.25          |
| (1,41) | 1:25:A:ASP:C | 1:26:A:ILE:N  | 1:26:A:ILE:CA | 1:26:A:ILE:C | 16       | 2.17          |
| (1,38) | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:ASP:N | 4        | 2.16          |
| (1,38) | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:ASP:N | 19       | 2.11          |
| (1,38) | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:ASP:N | 12       | 2.1           |
| (1,46) | 1:28:A:THR:N | 1:28:A:THR:CA | 1:28:A:THR:C  | 1:29:A:GLU:N | 16       | 2.09          |
| (1,38) | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:ASP:N | 10       | 2.09          |
| (1,44) | 1:27:A:ASP:N | 1:27:A:ASP:CA | 1:27:A:ASP:C  | 1:28:A:THR:N | 1        | 2.03          |
| (1,44) | 1:27:A:ASP:N | 1:27:A:ASP:CA | 1:27:A:ASP:C  | 1:28:A:THR:N | 12       | 2.02          |
| (1,38) | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:ASP:N | 2        | 2.02          |
| (1,38) | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:ASP:N | 3        | 1.99          |
| (1,38) | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:ASP:N | 20       | 1.99          |
| (1,38) | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:ASP:N | 8        | 1.96          |
| (1,91) | 1:58:A:HIS:N | 1:58:A:HIS:CA | 1:58:A:HIS:C  | 1:59:A:LEU:N | 8        | 1.89          |
| (1,88) | 1:56:A:ASN:C | 1:57:A:ILE:N  | 1:57:A:ILE:CA | 1:57:A:ILE:C | 5        | 1.88          |
| (1,91) | 1:58:A:HIS:N | 1:58:A:HIS:CA | 1:58:A:HIS:C  | 1:59:A:LEU:N | 20       | 1.86          |
| (1,38) | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:ASP:N | 5        | 1.86          |
| (1,44) | 1:27:A:ASP:N | 1:27:A:ASP:CA | 1:27:A:ASP:C  | 1:28:A:THR:N | 18       | 1.83          |
| (1,41) | 1:25:A:ASP:C | 1:26:A:ILE:N  | 1:26:A:ILE:CA | 1:26:A:ILE:C | 20       | 1.83          |
| (1,38) | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:ASP:N | 1        | 1.8           |
| (1,91) | 1:58:A:HIS:N | 1:58:A:HIS:CA | 1:58:A:HIS:C  | 1:59:A:LEU:N | 4        | 1.78          |
| (1,38) | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:ASP:N | 13       | 1.77          |
| (1,44) | 1:27:A:ASP:N | 1:27:A:ASP:CA | 1:27:A:ASP:C  | 1:28:A:THR:N | 13       | 1.76          |
| (1,91) | 1:58:A:HIS:N | 1:58:A:HIS:CA | 1:58:A:HIS:C  | 1:59:A:LEU:N | 12       | 1.75          |
| (1,91) | 1:58:A:HIS:N | 1:58:A:HIS:CA | 1:58:A:HIS:C  | 1:59:A:LEU:N | 3        | 1.74          |
| (1,41) | 1:25:A:ASP:C | 1:26:A:ILE:N  | 1:26:A:ILE:CA | 1:26:A:ILE:C | 15       | 1.73          |
| (1,40) | 1:25:A:ASP:N | 1:25:A:ASP:CA | 1:25:A:ASP:C  | 1:26:A:ILE:N | 2        | 1.73          |
| (1,44) | 1:27:A:ASP:N | 1:27:A:ASP:CA | 1:27:A:ASP:C  | 1:28:A:THR:N | 5        | 1.71          |
| (1,41) | 1:25:A:ASP:C | 1:26:A:ILE:N  | 1:26:A:ILE:CA | 1:26:A:ILE:C | 3        | 1.71          |

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*Continued from previous page...*

| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,41) | 1:25:A:ASP:C | 1:26:A:ILE:N  | 1:26:A:ILE:CA | 1:26:A:ILE:C | 19       | 1.71          |
| (1,44) | 1:27:A:ASP:N | 1:27:A:ASP:CA | 1:27:A:ASP:C  | 1:28:A:THR:N | 9        | 1.65          |
| (1,91) | 1:58:A:HIS:N | 1:58:A:HIS:CA | 1:58:A:HIS:C  | 1:59:A:LEU:N | 5        | 1.64          |
| (1,91) | 1:58:A:HIS:N | 1:58:A:HIS:CA | 1:58:A:HIS:C  | 1:59:A:LEU:N | 6        | 1.63          |
| (1,41) | 1:25:A:ASP:C | 1:26:A:ILE:N  | 1:26:A:ILE:CA | 1:26:A:ILE:C | 10       | 1.63          |
| (1,41) | 1:25:A:ASP:C | 1:26:A:ILE:N  | 1:26:A:ILE:CA | 1:26:A:ILE:C | 4        | 1.61          |
| (1,38) | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:ASP:N | 7        | 1.57          |
| (1,46) | 1:28:A:THR:N | 1:28:A:THR:CA | 1:28:A:THR:C  | 1:29:A:GLU:N | 5        | 1.56          |
| (1,38) | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:ASP:N | 15       | 1.54          |
| (1,38) | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:ASP:N | 18       | 1.53          |
| (1,97) | 1:61:A:ALA:N | 1:61:A:ALA:CA | 1:61:A:ALA:C  | 1:62:A:GLU:N | 17       | 1.5           |
| (1,44) | 1:27:A:ASP:N | 1:27:A:ASP:CA | 1:27:A:ASP:C  | 1:28:A:THR:N | 7        | 1.49          |
| (1,38) | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:ASP:N | 14       | 1.46          |
| (1,38) | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:ASP:N | 11       | 1.44          |
| (1,38) | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:ASP:N | 17       | 1.43          |
| (1,97) | 1:61:A:ALA:N | 1:61:A:ALA:CA | 1:61:A:ALA:C  | 1:62:A:GLU:N | 2        | 1.38          |
| (1,88) | 1:56:A:ASN:C | 1:57:A:ILE:N  | 1:57:A:ILE:CA | 1:57:A:ILE:C | 10       | 1.38          |
| (1,46) | 1:28:A:THR:N | 1:28:A:THR:CA | 1:28:A:THR:C  | 1:29:A:GLU:N | 4        | 1.38          |
| (1,91) | 1:58:A:HIS:N | 1:58:A:HIS:CA | 1:58:A:HIS:C  | 1:59:A:LEU:N | 11       | 1.36          |
| (1,91) | 1:58:A:HIS:N | 1:58:A:HIS:CA | 1:58:A:HIS:C  | 1:59:A:LEU:N | 13       | 1.36          |
| (1,91) | 1:58:A:HIS:N | 1:58:A:HIS:CA | 1:58:A:HIS:C  | 1:59:A:LEU:N | 18       | 1.36          |
| (1,97) | 1:61:A:ALA:N | 1:61:A:ALA:CA | 1:61:A:ALA:C  | 1:62:A:GLU:N | 12       | 1.35          |
| (1,38) | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:ASP:N | 9        | 1.35          |
| (1,81) | 1:53:A:LYS:N | 1:53:A:LYS:CA | 1:53:A:LYS:C  | 1:54:A:ARG:N | 16       | 1.27          |
| (1,81) | 1:53:A:LYS:N | 1:53:A:LYS:CA | 1:53:A:LYS:C  | 1:54:A:ARG:N | 10       | 1.25          |
| (1,97) | 1:61:A:ALA:N | 1:61:A:ALA:CA | 1:61:A:ALA:C  | 1:62:A:GLU:N | 10       | 1.23          |
| (1,91) | 1:58:A:HIS:N | 1:58:A:HIS:CA | 1:58:A:HIS:C  | 1:59:A:LEU:N | 2        | 1.23          |
| (1,39) | 1:24:A:ALA:C | 1:25:A:ASP:N  | 1:25:A:ASP:CA | 1:25:A:ASP:C | 6        | 1.22          |
| (1,81) | 1:53:A:LYS:N | 1:53:A:LYS:CA | 1:53:A:LYS:C  | 1:54:A:ARG:N | 18       | 1.19          |
| (1,44) | 1:27:A:ASP:N | 1:27:A:ASP:CA | 1:27:A:ASP:C  | 1:28:A:THR:N | 19       | 1.16          |
| (1,97) | 1:61:A:ALA:N | 1:61:A:ALA:CA | 1:61:A:ALA:C  | 1:62:A:GLU:N | 11       | 1.14          |
| (1,91) | 1:58:A:HIS:N | 1:58:A:HIS:CA | 1:58:A:HIS:C  | 1:59:A:LEU:N | 16       | 1.14          |
| (1,94) | 1:59:A:LEU:C | 1:60:A:ASN:N  | 1:60:A:ASN:CA | 1:60:A:ASN:C | 5        | 1.13          |
| (1,88) | 1:56:A:ASN:C | 1:57:A:ILE:N  | 1:57:A:ILE:CA | 1:57:A:ILE:C | 18       | 1.12          |
| (1,38) | 1:24:A:ALA:N | 1:24:A:ALA:CA | 1:24:A:ALA:C  | 1:25:A:ASP:N | 16       | 1.11          |
| (1,94) | 1:59:A:LEU:C | 1:60:A:ASN:N  | 1:60:A:ASN:CA | 1:60:A:ASN:C | 6        | 1.1           |
| (1,91) | 1:58:A:HIS:N | 1:58:A:HIS:CA | 1:58:A:HIS:C  | 1:59:A:LEU:N | 1        | 1.09          |
| (1,88) | 1:56:A:ASN:C | 1:57:A:ILE:N  | 1:57:A:ILE:CA | 1:57:A:ILE:C | 6        | 1.08          |
| (1,85) | 1:55:A:TYR:N | 1:55:A:TYR:CA | 1:55:A:TYR:C  | 1:56:A:ASN:N | 9        | 1.07          |
| (1,85) | 1:55:A:TYR:N | 1:55:A:TYR:CA | 1:55:A:TYR:C  | 1:56:A:ASN:N | 15       | 1.06          |
| (1,46) | 1:28:A:THR:N | 1:28:A:THR:CA | 1:28:A:THR:C  | 1:29:A:GLU:N | 10       | 1.04          |
| (1,41) | 1:25:A:ASP:C | 1:26:A:ILE:N  | 1:26:A:ILE:CA | 1:26:A:ILE:C | 2        | 1.04          |