



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 09:03 AM UTC

PDB ID : 2JPI / pdb\_00002jpi  
BMRB ID : 15246  
Title : NMR structure of PA4090 from *Pseudomonas aeruginosa*  
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Deposited on : 2007-05-13

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

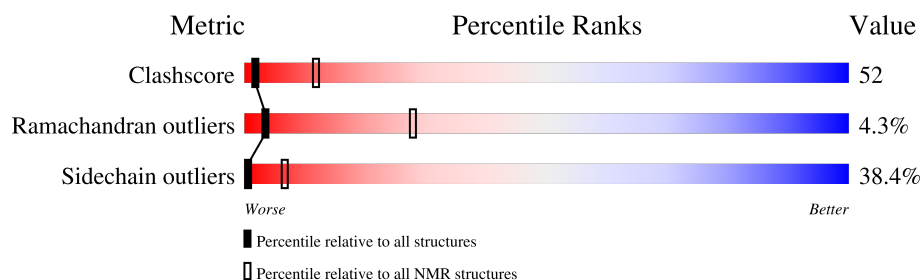
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 81%.

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



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

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 118    |                  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 11 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:1-A:39, A:44-A:81, A:87-A:94 (85) | 0.20              | 11           |

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1503 atoms, of which 731 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Hypothetical protein.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 96       | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1503  | 478 | 731 | 140 | 148 | 6 |       |

There are 22 discrepancies between the modelled and reference sequences:

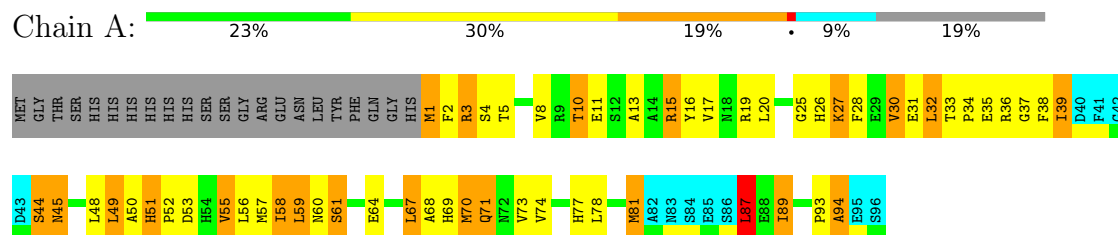
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -21     | MET      | -      | expression tag | UNP Q9HWT8 |
| A     | -20     | GLY      | -      | expression tag | UNP Q9HWT8 |
| A     | -19     | THR      | -      | expression tag | UNP Q9HWT8 |
| A     | -18     | SER      | -      | expression tag | UNP Q9HWT8 |
| A     | -17     | HIS      | -      | expression tag | UNP Q9HWT8 |
| A     | -16     | HIS      | -      | expression tag | UNP Q9HWT8 |
| A     | -15     | HIS      | -      | expression tag | UNP Q9HWT8 |
| A     | -14     | HIS      | -      | expression tag | UNP Q9HWT8 |
| A     | -13     | HIS      | -      | expression tag | UNP Q9HWT8 |
| A     | -12     | HIS      | -      | expression tag | UNP Q9HWT8 |
| A     | -11     | SER      | -      | expression tag | UNP Q9HWT8 |
| A     | -10     | SER      | -      | expression tag | UNP Q9HWT8 |
| A     | -9      | GLY      | -      | expression tag | UNP Q9HWT8 |
| A     | -8      | ARG      | -      | expression tag | UNP Q9HWT8 |
| A     | -7      | GLU      | -      | expression tag | UNP Q9HWT8 |
| A     | -6      | ASN      | -      | expression tag | UNP Q9HWT8 |
| A     | -5      | LEU      | -      | expression tag | UNP Q9HWT8 |
| A     | -4      | TYR      | -      | expression tag | UNP Q9HWT8 |
| A     | -3      | PHE      | -      | expression tag | UNP Q9HWT8 |
| A     | -2      | GLN      | -      | expression tag | UNP Q9HWT8 |
| A     | -1      | GLY      | -      | expression tag | UNP Q9HWT8 |
| A     | 0       | HIS      | -      | expression tag | UNP Q9HWT8 |

## 4 Residue-property plots

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

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

- Molecule 1: Hypothetical protein

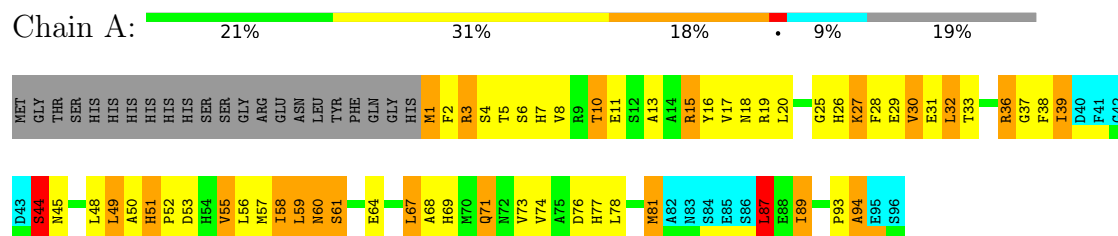


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: Hypothetical protein



#### 4.2.2 Score per residue for model 2

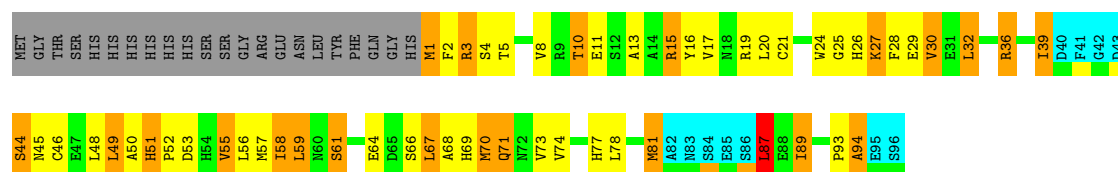
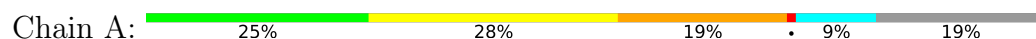
- Molecule 1: Hypothetical protein





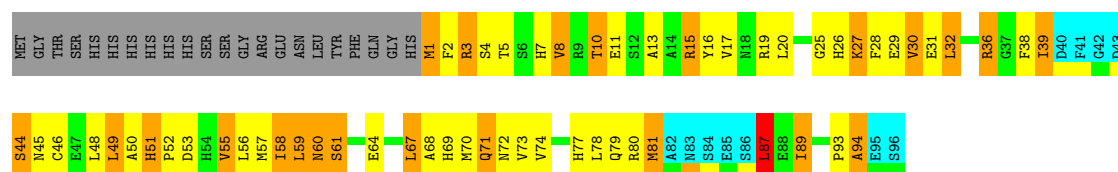
### 4.2.3 Score per residue for model 3

- Molecule 1: Hypothetical protein



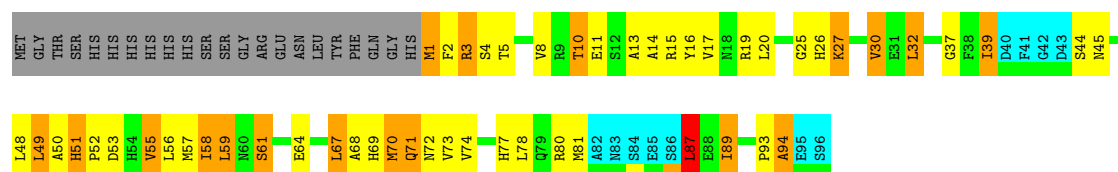
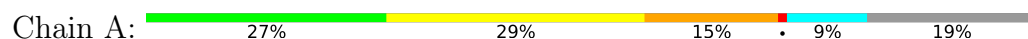
### 4.2.4 Score per residue for model 4

- Molecule 1: Hypothetical protein



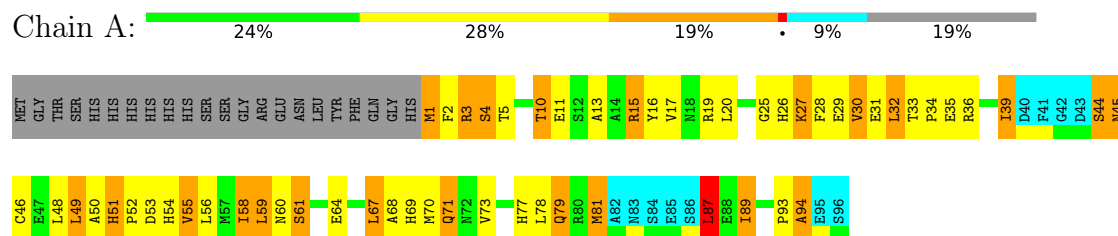
### 4.2.5 Score per residue for model 5

- Molecule 1: Hypothetical protein



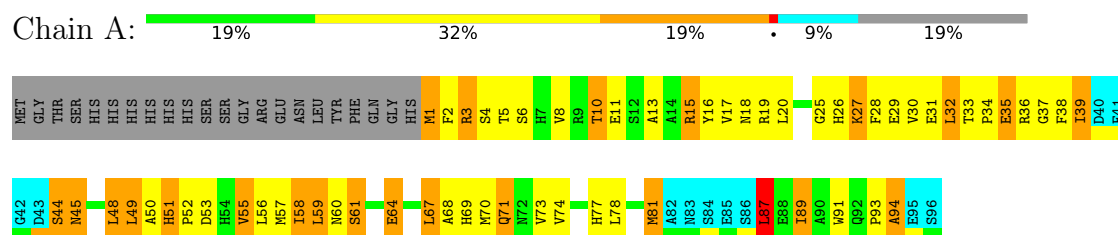
### 4.2.6 Score per residue for model 6

- Molecule 1: Hypothetical protein



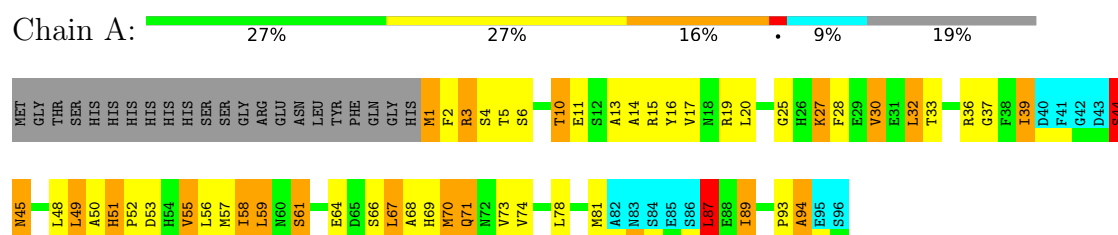
#### 4.2.7 Score per residue for model 7

- Molecule 1: Hypothetical protein



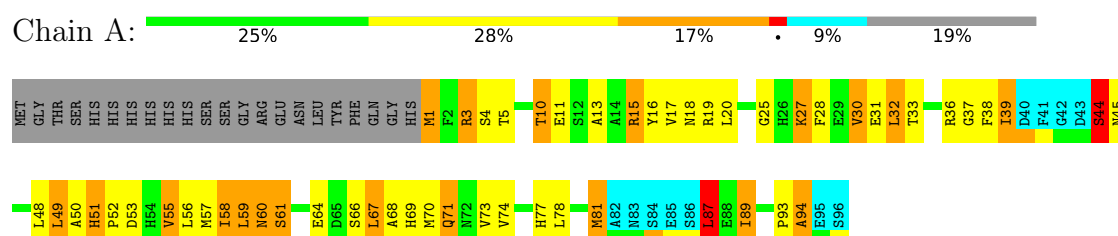
#### 4.2.8 Score per residue for model 8

- Molecule 1: Hypothetical protein



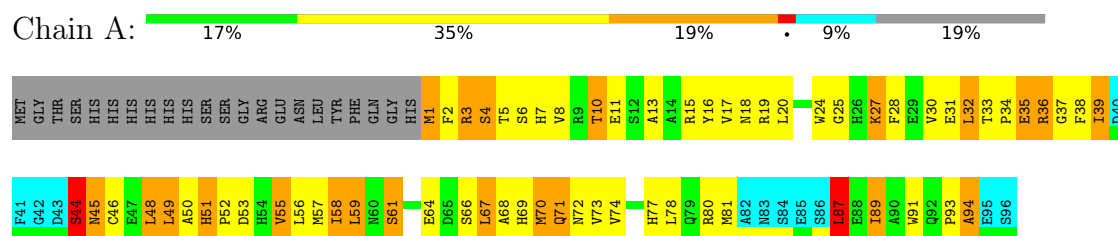
#### 4.2.9 Score per residue for model 9

- Molecule 1: Hypothetical protein



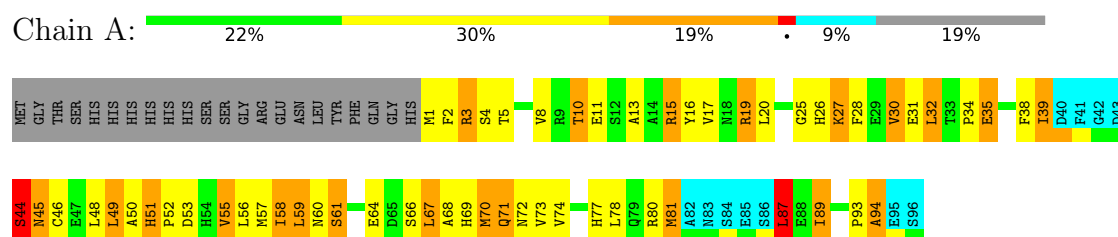
### 4.2.10 Score per residue for model 10

- Molecule 1: Hypothetical protein



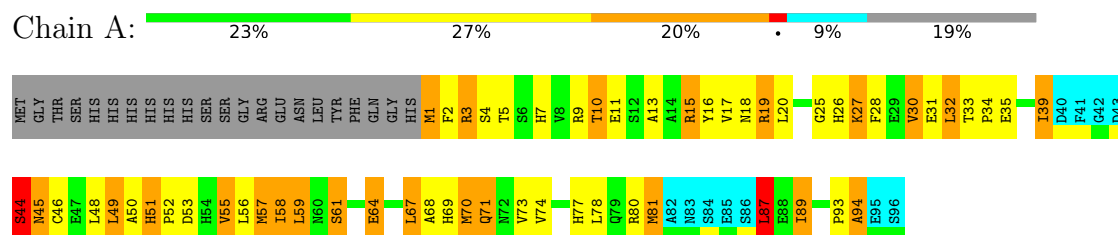
### 4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Hypothetical protein



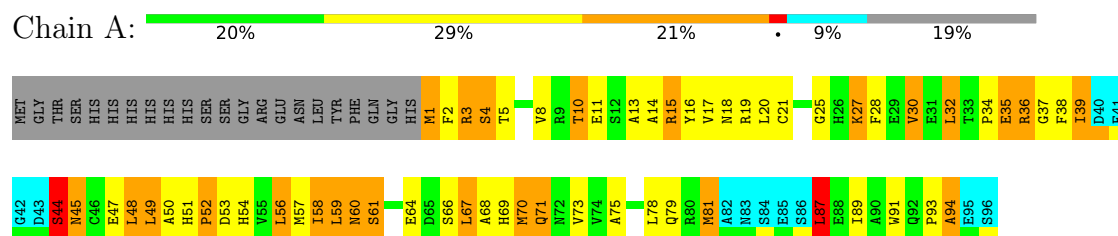
### 4.2.12 Score per residue for model 12

- Molecule 1: Hypothetical protein



### 4.2.13 Score per residue for model 13

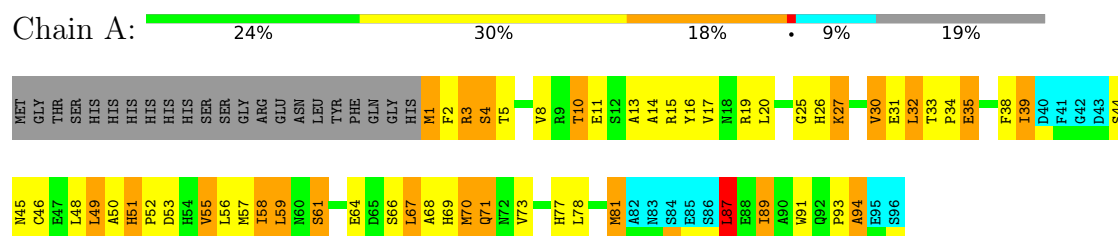
- Molecule 1: Hypothetical protein





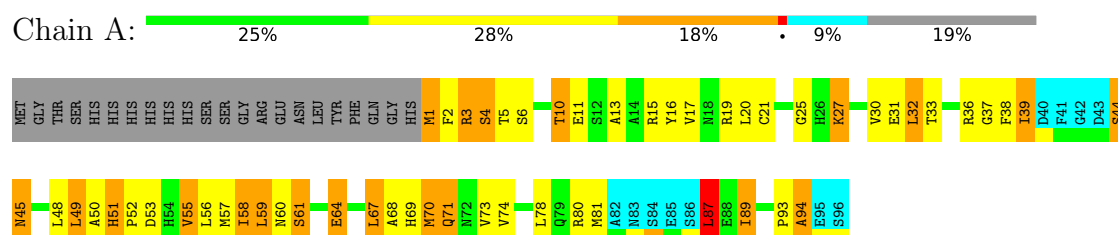
## 4.2.18 Score per residue for model 18

- Molecule 1: Hypothetical protein



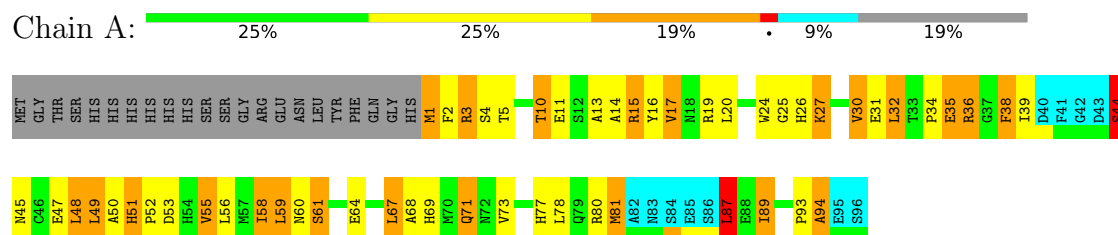
## 4.2.19 Score per residue for model 19

- Molecule 1: Hypothetical protein



## 4.2.20 Score per residue for model 20

- Molecule 1: Hypothetical protein



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification | Version |
|---------------|----------------|---------|
| CNS           | refinement     | 1.1     |

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                       | 1041           |
| Number of shifts mapped to atoms             | 1041           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 81%            |

## 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     | 691   | 673      | 669      | 70±6    |
| All | All   | 13820 | 13460    | 13380    | 1405    |

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 52.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:5:THR:HG22  | 1:A:58:ILE:HD13 | 0.90     | 1.43        | 4      | 20    |
| 1:A:10:THR:OG1  | 1:A:81:MET:HE1  | 0.86     | 1.70        | 13     | 20    |
| 1:A:16:TYR:O    | 1:A:20:LEU:HG   | 0.84     | 1.72        | 16     | 20    |
| 1:A:67:LEU:HD11 | 1:A:94:ALA:HB3  | 0.82     | 1.50        | 4      | 20    |
| 1:A:67:LEU:HD11 | 1:A:94:ALA:CB   | 0.82     | 2.03        | 7      | 20    |
| 1:A:59:LEU:HD22 | 1:A:59:LEU:C    | 0.80     | 2.01        | 6      | 20    |
| 1:A:48:LEU:HD23 | 1:A:48:LEU:N    | 0.80     | 1.91        | 13     | 6     |
| 1:A:69:HIS:O    | 1:A:73:VAL:HG23 | 0.78     | 1.78        | 15     | 20    |
| 1:A:59:LEU:HD22 | 1:A:59:LEU:O    | 0.76     | 1.81        | 3      | 20    |
| 1:A:59:LEU:HD23 | 1:A:61:SER:OG   | 0.76     | 1.80        | 4      | 19    |
| 1:A:67:LEU:HD23 | 1:A:68:ALA:N    | 0.73     | 1.98        | 14     | 20    |
| 1:A:6:SER:HB3   | 1:A:57:MET:HE3  | 0.72     | 1.61        | 15     | 6     |
| 1:A:67:LEU:C    | 1:A:67:LEU:HD23 | 0.72     | 2.10        | 16     | 18    |
| 1:A:6:SER:CB    | 1:A:57:MET:HE3  | 0.71     | 2.16        | 10     | 6     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:64:GLU:HA   | 1:A:67:LEU:HB3  | 0.71     | 1.63        | 15     | 20    |
| 1:A:25:GLY:HA3  | 1:A:30:VAL:HG21 | 0.70     | 1.63        | 20     | 20    |
| 1:A:67:LEU:HD23 | 1:A:67:LEU:C    | 0.70     | 2.11        | 19     | 2     |
| 1:A:3:ARG:HG3   | 1:A:59:LEU:O    | 0.68     | 1.88        | 2      | 20    |
| 1:A:78:LEU:HD22 | 1:A:81:MET:HE3  | 0.68     | 1.64        | 4      | 15    |
| 1:A:30:VAL:CG1  | 1:A:39:ILE:HG23 | 0.67     | 2.19        | 19     | 3     |
| 1:A:4:SER:CB    | 1:A:94:ALA:HB2  | 0.67     | 2.20        | 13     | 20    |
| 1:A:59:LEU:HD12 | 1:A:71:GLN:HB3  | 0.66     | 1.68        | 2      | 1     |
| 1:A:4:SER:HB2   | 1:A:94:ALA:HB2  | 0.66     | 1.66        | 13     | 20    |
| 1:A:5:THR:CG2   | 1:A:58:ILE:HD13 | 0.66     | 2.19        | 4      | 20    |
| 1:A:55:VAL:HG11 | 1:A:78:LEU:HD11 | 0.64     | 1.69        | 6      | 18    |
| 1:A:64:GLU:HG3  | 1:A:67:LEU:HD13 | 0.64     | 1.69        | 9      | 16    |
| 1:A:10:THR:HG22 | 1:A:13:ALA:HB2  | 0.64     | 1.69        | 6      | 20    |
| 1:A:51:HIS:CG   | 1:A:52:PRO:HD2  | 0.64     | 2.28        | 20     | 19    |
| 1:A:17:VAL:CG2  | 1:A:50:ALA:HB2  | 0.63     | 2.23        | 13     | 11    |
| 1:A:13:ALA:C    | 1:A:50:ALA:HB1  | 0.63     | 2.18        | 6      | 20    |
| 1:A:20:LEU:HD12 | 1:A:48:LEU:HD11 | 0.63     | 1.69        | 10     | 6     |
| 1:A:49:LEU:HB3  | 1:A:56:LEU:HB2  | 0.61     | 1.72        | 2      | 20    |
| 1:A:87:LEU:HD12 | 1:A:89:ILE:CG2  | 0.61     | 2.25        | 8      | 20    |
| 1:A:59:LEU:C    | 1:A:59:LEU:CD2  | 0.61     | 2.73        | 3      | 19    |
| 1:A:30:VAL:HG12 | 1:A:39:ILE:HG12 | 0.61     | 1.73        | 15     | 17    |
| 1:A:93:PRO:O    | 1:A:94:ALA:HB3  | 0.60     | 1.96        | 6      | 20    |
| 1:A:6:SER:OG    | 1:A:57:MET:HE3  | 0.59     | 1.97        | 1      | 5     |
| 1:A:89:ILE:O    | 1:A:89:ILE:HG12 | 0.58     | 1.98        | 5      | 19    |
| 1:A:93:PRO:O    | 1:A:94:ALA:CB   | 0.57     | 2.51        | 2      | 20    |
| 1:A:48:LEU:HD12 | 1:A:56:LEU:O    | 0.57     | 1.99        | 15     | 13    |
| 1:A:13:ALA:HB3  | 1:A:51:HIS:O    | 0.57     | 1.99        | 14     | 19    |
| 1:A:4:SER:HB3   | 1:A:59:LEU:HD11 | 0.57     | 1.75        | 2      | 1     |
| 1:A:48:LEU:N    | 1:A:48:LEU:CD2  | 0.57     | 2.65        | 13     | 6     |
| 1:A:66:SER:O    | 1:A:70:MET:HG2  | 0.56     | 2.00        | 18     | 8     |
| 1:A:59:LEU:CD2  | 1:A:59:LEU:C    | 0.56     | 2.78        | 2      | 1     |
| 1:A:32:LEU:C    | 1:A:32:LEU:CD2  | 0.56     | 2.79        | 11     | 20    |
| 1:A:67:LEU:C    | 1:A:67:LEU:CD2  | 0.55     | 2.80        | 9      | 20    |
| 1:A:30:VAL:HG13 | 1:A:39:ILE:HG23 | 0.55     | 1.78        | 1      | 12    |
| 1:A:67:LEU:CD2  | 1:A:68:ALA:N    | 0.55     | 2.68        | 14     | 20    |
| 1:A:30:VAL:HA   | 1:A:38:PHE:O    | 0.54     | 2.02        | 10     | 4     |
| 1:A:70:MET:N    | 1:A:70:MET:HE3  | 0.54     | 2.18        | 14     | 1     |
| 1:A:25:GLY:CA   | 1:A:30:VAL:HG21 | 0.54     | 2.33        | 15     | 20    |
| 1:A:78:LEU:HB3  | 1:A:87:LEU:HD11 | 0.54     | 1.77        | 13     | 19    |
| 1:A:17:VAL:HG11 | 1:A:36:ARG:HA   | 0.54     | 1.78        | 16     | 12    |
| 1:A:17:VAL:HG23 | 1:A:50:ALA:HB2  | 0.54     | 1.80        | 10     | 14    |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:51:HIS:CD2  | 1:A:52:PRO:HD2  | 0.54     | 2.37        | 13     | 1     |
| 1:A:59:LEU:HB2  | 1:A:70:MET:HB2  | 0.54     | 1.79        | 18     | 17    |
| 1:A:44:SER:OG   | 1:A:70:MET:HE3  | 0.54     | 2.03        | 9      | 1     |
| 1:A:15:ARG:CD   | 1:A:19:ARG:HD2  | 0.54     | 2.33        | 16     | 1     |
| 1:A:15:ARG:C    | 1:A:15:ARG:HD2  | 0.54     | 2.28        | 14     | 7     |
| 1:A:1:MET:O     | 1:A:1:MET:HG3   | 0.54     | 2.03        | 6      | 7     |
| 1:A:10:THR:O    | 1:A:53:ASP:C    | 0.53     | 2.52        | 12     | 20    |
| 1:A:68:ALA:HA   | 1:A:71:GLN:CG   | 0.53     | 2.34        | 5      | 20    |
| 1:A:51:HIS:O    | 1:A:53:ASP:N    | 0.52     | 2.42        | 13     | 1     |
| 1:A:21:CYS:SG   | 1:A:32:LEU:HD12 | 0.52     | 2.45        | 13     | 5     |
| 1:A:24:TRP:CH2  | 1:A:77:HIS:CE1  | 0.51     | 2.99        | 3      | 1     |
| 1:A:68:ALA:HA   | 1:A:71:GLN:HG3  | 0.51     | 1.83        | 16     | 20    |
| 1:A:59:LEU:H    | 1:A:59:LEU:HD13 | 0.51     | 1.66        | 2      | 1     |
| 1:A:1:MET:HG2   | 1:A:1:MET:O     | 0.51     | 2.05        | 7      | 13    |
| 1:A:15:ARG:NE   | 1:A:19:ARG:CD   | 0.51     | 2.74        | 16     | 1     |
| 1:A:48:LEU:HD22 | 1:A:74:VAL:HG13 | 0.51     | 1.83        | 19     | 8     |
| 1:A:91:TRP:CD1  | 1:A:91:TRP:O    | 0.51     | 2.64        | 10     | 3     |
| 1:A:55:VAL:HG11 | 1:A:78:LEU:CD1  | 0.50     | 2.36        | 10     | 16    |
| 1:A:32:LEU:C    | 1:A:32:LEU:HD23 | 0.50     | 2.32        | 20     | 7     |
| 1:A:17:VAL:CG1  | 1:A:37:GLY:N    | 0.50     | 2.75        | 17     | 6     |
| 1:A:16:TYR:CD2  | 1:A:81:MET:HE2  | 0.50     | 2.42        | 4      | 7     |
| 1:A:81:MET:C    | 1:A:81:MET:SD   | 0.50     | 2.95        | 19     | 8     |
| 1:A:20:LEU:HD22 | 1:A:24:TRP:CZ3  | 0.49     | 2.42        | 3      | 1     |
| 1:A:17:VAL:HG22 | 1:A:48:LEU:HG   | 0.49     | 1.84        | 3      | 11    |
| 1:A:57:MET:SD   | 1:A:74:VAL:HG12 | 0.49     | 2.47        | 17     | 16    |
| 1:A:51:HIS:CG   | 1:A:52:PRO:CD   | 0.49     | 2.95        | 20     | 18    |
| 1:A:18:ASN:ND2  | 1:A:32:LEU:HD21 | 0.49     | 2.22        | 9      | 3     |
| 1:A:34:PRO:O    | 1:A:35:GLU:CG   | 0.49     | 2.61        | 2      | 11    |
| 1:A:36:ARG:CB   | 1:A:48:LEU:O    | 0.48     | 2.60        | 13     | 11    |
| 1:A:38:PHE:CE1  | 1:A:45:ASN:ND2  | 0.48     | 2.81        | 7      | 1     |
| 1:A:51:HIS:CG   | 1:A:54:HIS:NE2  | 0.48     | 2.81        | 13     | 1     |
| 1:A:17:VAL:CG2  | 1:A:48:LEU:HG   | 0.48     | 2.39        | 8      | 14    |
| 1:A:36:ARG:HA   | 1:A:48:LEU:O    | 0.48     | 2.08        | 16     | 7     |
| 1:A:5:THR:HG22  | 1:A:58:ILE:CD1  | 0.48     | 2.30        | 3      | 17    |
| 1:A:66:SER:O    | 1:A:70:MET:HE2  | 0.47     | 2.08        | 9      | 1     |
| 1:A:48:LEU:HD11 | 1:A:55:VAL:HG22 | 0.47     | 1.86        | 18     | 5     |
| 1:A:27:LYS:O    | 1:A:27:LYS:CG   | 0.47     | 2.62        | 7      | 20    |
| 1:A:45:ASN:N    | 1:A:60:ASN:O    | 0.47     | 2.48        | 2      | 8     |
| 1:A:44:SER:OG   | 1:A:45:ASN:N    | 0.47     | 2.47        | 2      | 5     |
| 1:A:16:TYR:HD2  | 1:A:81:MET:HE2  | 0.47     | 1.70        | 17     | 3     |
| 1:A:36:ARG:HE   | 1:A:49:LEU:HD12 | 0.47     | 1.69        | 20     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:16:TYR:CE2  | 1:A:81:MET:HB2  | 0.46     | 2.45        | 11     | 18    |
| 1:A:55:VAL:CG1  | 1:A:78:LEU:HD11 | 0.46     | 2.40        | 5      | 16    |
| 1:A:10:THR:CG2  | 1:A:13:ALA:HB2  | 0.46     | 2.39        | 10     | 12    |
| 1:A:78:LEU:CB   | 1:A:87:LEU:HD11 | 0.46     | 2.40        | 5      | 3     |
| 1:A:49:LEU:O    | 1:A:55:VAL:CG2  | 0.46     | 2.63        | 5      | 19    |
| 1:A:16:TYR:CZ   | 1:A:81:MET:CB   | 0.46     | 2.99        | 6      | 1     |
| 1:A:34:PRO:O    | 1:A:35:GLU:HG2  | 0.46     | 2.11        | 7      | 1     |
| 1:A:51:HIS:CB   | 1:A:54:HIS:CE1  | 0.46     | 2.99        | 13     | 1     |
| 1:A:17:VAL:HG22 | 1:A:48:LEU:HD12 | 0.46     | 1.87        | 10     | 6     |
| 1:A:24:TRP:CH2  | 1:A:77:HIS:NE2  | 0.46     | 2.84        | 3      | 1     |
| 1:A:30:VAL:HG12 | 1:A:39:ILE:HG23 | 0.45     | 1.87        | 10     | 1     |
| 1:A:59:LEU:HD13 | 1:A:59:LEU:N    | 0.45     | 2.26        | 2      | 1     |
| 1:A:61:SER:OG   | 1:A:67:LEU:HA   | 0.45     | 2.11        | 2      | 1     |
| 1:A:16:TYR:CE2  | 1:A:81:MET:HE2  | 0.45     | 2.46        | 11     | 5     |
| 1:A:24:TRP:NE1  | 1:A:77:HIS:CE1  | 0.45     | 2.85        | 20     | 1     |
| 1:A:17:VAL:CG2  | 1:A:50:ALA:CB   | 0.45     | 2.95        | 6      | 16    |
| 1:A:44:SER:C    | 1:A:45:ASN:CG   | 0.45     | 2.85        | 17     | 1     |
| 1:A:18:ASN:CG   | 1:A:32:LEU:HD21 | 0.45     | 2.37        | 7      | 6     |
| 1:A:29:GLU:O    | 1:A:29:GLU:HG3  | 0.45     | 2.12        | 7      | 1     |
| 1:A:51:HIS:CD2  | 1:A:52:PRO:CD   | 0.44     | 2.99        | 13     | 1     |
| 1:A:46:CYS:SG   | 1:A:74:VAL:HG23 | 0.44     | 2.52        | 10     | 2     |
| 1:A:15:ARG:NE   | 1:A:19:ARG:HD2  | 0.44     | 2.27        | 16     | 1     |
| 1:A:15:ARG:O    | 1:A:15:ARG:CD   | 0.44     | 2.66        | 9      | 6     |
| 1:A:17:VAL:HG13 | 1:A:37:GLY:N    | 0.44     | 2.28        | 9      | 5     |
| 1:A:38:PHE:CE2  | 1:A:47:GLU:CD   | 0.44     | 2.96        | 20     | 1     |
| 1:A:44:SER:C    | 1:A:45:ASN:ND2  | 0.43     | 2.76        | 8      | 5     |
| 1:A:15:ARG:NE   | 1:A:19:ARG:HD3  | 0.43     | 2.28        | 11     | 2     |
| 1:A:19:ARG:O    | 1:A:23:HIS:ND1  | 0.43     | 2.51        | 17     | 1     |
| 1:A:81:MET:SD   | 1:A:81:MET:C    | 0.43     | 3.02        | 8      | 2     |
| 1:A:18:ASN:OD1  | 1:A:32:LEU:HD21 | 0.43     | 2.14        | 14     | 1     |
| 1:A:15:ARG:CZ   | 1:A:19:ARG:HD2  | 0.43     | 2.43        | 15     | 1     |
| 1:A:27:LYS:O    | 1:A:27:LYS:HE3  | 0.43     | 2.14        | 15     | 3     |
| 1:A:30:VAL:HG12 | 1:A:39:ILE:CG1  | 0.43     | 2.43        | 4      | 6     |
| 1:A:87:LEU:HD12 | 1:A:89:ILE:HG21 | 0.43     | 1.90        | 8      | 4     |
| 1:A:36:ARG:CA   | 1:A:48:LEU:O    | 0.43     | 2.67        | 2      | 6     |
| 1:A:17:VAL:HG11 | 1:A:36:ARG:CA   | 0.43     | 2.43        | 16     | 1     |
| 1:A:4:SER:HB2   | 1:A:94:ALA:CB   | 0.42     | 2.42        | 19     | 14    |
| 1:A:87:LEU:CD1  | 1:A:89:ILE:CG2  | 0.42     | 2.96        | 2      | 7     |
| 1:A:24:TRP:O    | 1:A:24:TRP:CD1  | 0.42     | 2.72        | 10     | 1     |
| 1:A:16:TYR:CE2  | 1:A:81:MET:CB   | 0.42     | 3.02        | 6      | 1     |
| 1:A:7:HIS:CD2   | 1:A:9:ARG:NH1   | 0.42     | 2.87        | 16     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:19:ARG:NH2  | 1:A:32:LEU:HD11 | 0.42     | 2.30        | 16     | 1     |
| 1:A:27:LYS:O    | 1:A:27:LYS:CD   | 0.42     | 2.67        | 20     | 1     |
| 1:A:8:VAL:CG2   | 1:A:57:MET:HE2  | 0.42     | 2.44        | 5      | 1     |
| 1:A:59:LEU:HG   | 1:A:67:LEU:O    | 0.42     | 2.15        | 16     | 4     |
| 1:A:64:GLU:CA   | 1:A:67:LEU:HB3  | 0.42     | 2.42        | 8      | 6     |
| 1:A:73:VAL:O    | 1:A:77:HIS:CE1  | 0.42     | 2.72        | 17     | 15    |
| 1:A:45:ASN:OD1  | 1:A:45:ASN:N    | 0.42     | 2.53        | 19     | 1     |
| 1:A:38:PHE:CE1  | 1:A:45:ASN:OD1  | 0.42     | 2.73        | 4      | 1     |
| 1:A:44:SER:C    | 1:A:45:ASN:OD1  | 0.42     | 2.63        | 13     | 1     |
| 1:A:79:GLN:HA   | 1:A:87:LEU:HD23 | 0.42     | 1.92        | 6      | 1     |
| 1:A:44:SER:O    | 1:A:45:ASN:CG   | 0.42     | 2.63        | 9      | 1     |
| 1:A:24:TRP:CZ2  | 1:A:28:PHE:CE1  | 0.42     | 3.08        | 10     | 1     |
| 1:A:27:LYS:O    | 1:A:27:LYS:CE   | 0.41     | 2.67        | 17     | 6     |
| 1:A:30:VAL:CG1  | 1:A:39:ILE:HD13 | 0.41     | 2.44        | 9      | 1     |
| 1:A:44:SER:HA   | 1:A:60:ASN:O    | 0.41     | 2.15        | 9      | 1     |
| 1:A:7:HIS:CD2   | 1:A:7:HIS:C     | 0.41     | 2.98        | 4      | 4     |
| 1:A:8:VAL:CG2   | 1:A:57:MET:CE   | 0.41     | 2.99        | 13     | 8     |
| 1:A:44:SER:O    | 1:A:45:ASN:ND2  | 0.41     | 2.53        | 1      | 1     |
| 1:A:45:ASN:ND2  | 1:A:45:ASN:N    | 0.41     | 2.69        | 10     | 1     |
| 1:A:16:TYR:CZ   | 1:A:81:MET:HB2  | 0.41     | 2.51        | 6      | 1     |
| 1:A:47:GLU:C    | 1:A:48:LEU:HD23 | 0.41     | 2.38        | 13     | 1     |
| 1:A:91:TRP:O    | 1:A:91:TRP:CE3  | 0.41     | 2.74        | 7      | 2     |
| 1:A:75:ALA:O    | 1:A:79:GLN:CG   | 0.41     | 2.69        | 13     | 1     |
| 1:A:59:LEU:HD21 | 1:A:67:LEU:HG   | 0.41     | 1.92        | 20     | 2     |
| 1:A:48:LEU:HD13 | 1:A:74:VAL:HG11 | 0.41     | 1.92        | 15     | 1     |
| 1:A:59:LEU:CB   | 1:A:70:MET:HB2  | 0.41     | 2.46        | 16     | 2     |
| 1:A:49:LEU:O    | 1:A:55:VAL:HG22 | 0.41     | 2.17        | 5      | 1     |
| 1:A:78:LEU:CB   | 1:A:87:LEU:CD1  | 0.41     | 2.99        | 5      | 1     |
| 1:A:27:LYS:O    | 1:A:27:LYS:HG2  | 0.41     | 2.15        | 7      | 2     |
| 1:A:59:LEU:HD23 | 1:A:67:LEU:HA   | 0.40     | 1.94        | 16     | 2     |
| 1:A:7:HIS:CE1   | 1:A:9:ARG:NH1   | 0.40     | 2.89        | 12     | 1     |
| 1:A:51:HIS:HB2  | 1:A:54:HIS:CE1  | 0.40     | 2.51        | 6      | 1     |
| 1:A:21:CYS:SG   | 1:A:32:LEU:HB2  | 0.40     | 2.55        | 16     | 1     |
| 1:A:24:TRP:NE1  | 1:A:77:HIS:NE2  | 0.40     | 2.70        | 20     | 1     |
| 1:A:57:MET:SD   | 1:A:74:VAL:CG1  | 0.40     | 3.10        | 17     | 1     |
| 1:A:10:THR:O    | 1:A:53:ASP:HA   | 0.40     | 2.16        | 20     | 1     |
| 1:A:29:GLU:HG3  | 1:A:29:GLU:O    | 0.40     | 2.17        | 4      | 1     |
| 1:A:48:LEU:HD12 | 1:A:49:LEU:N    | 0.40     | 2.30        | 18     | 1     |
| 1:A:24:TRP:O    | 1:A:26:HIS:N    | 0.40     | 2.53        | 15     | 1     |

## 6.3 Torsion angles

### 6.3.1 Protein backbone

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

| Mol | Chain | Analysed        | Favoured     | Allowed     | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|-------------|------------|-------------|----|
| 1   | A     | 84/118 (71%)    | 72±1 (85±1%) | 9±1 (10±2%) | 4±1 (4±1%) | 3           | 28 |
| All | All   | 1680/2360 (71%) | 1433 (85%)   | 174 (10%)   | 73 (4%)    | 3           | 28 |

All 6 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 87  | LEU  | 20             |
| 1   | A     | 94  | ALA  | 20             |
| 1   | A     | 44  | SER  | 17             |
| 1   | A     | 35  | GLU  | 10             |
| 1   | A     | 14  | ALA  | 5              |
| 1   | A     | 52  | PRO  | 1              |

### 6.3.2 Protein sidechains

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

| Mol | Chain | Analysed        | Rotameric    | Outliers     | Percentiles |   |
|-----|-------|-----------------|--------------|--------------|-------------|---|
| 1   | A     | 76/104 (73%)    | 47±2 (62±3%) | 29±2 (38±3%) | 0           | 7 |
| All | All   | 1520/2080 (73%) | 936 (62%)    | 584 (38%)    | 0           | 7 |

All 49 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     | 3   | ARG  | 20             |
| 1   | A     | 10  | THR  | 20             |
| 1   | A     | 11  | GLU  | 20             |
| 1   | A     | 15  | ARG  | 20             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 19  | ARG  | 20             |
| 1   | A     | 27  | LYS  | 20             |
| 1   | A     | 32  | LEU  | 20             |
| 1   | A     | 39  | ILE  | 20             |
| 1   | A     | 49  | LEU  | 20             |
| 1   | A     | 58  | ILE  | 20             |
| 1   | A     | 59  | LEU  | 20             |
| 1   | A     | 61  | SER  | 20             |
| 1   | A     | 67  | LEU  | 20             |
| 1   | A     | 71  | GLN  | 20             |
| 1   | A     | 87  | LEU  | 20             |
| 1   | A     | 1   | MET  | 19             |
| 1   | A     | 2   | PHE  | 19             |
| 1   | A     | 51  | HIS  | 19             |
| 1   | A     | 55  | VAL  | 19             |
| 1   | A     | 89  | ILE  | 19             |
| 1   | A     | 30  | VAL  | 17             |
| 1   | A     | 44  | SER  | 16             |
| 1   | A     | 81  | MET  | 16             |
| 1   | A     | 45  | ASN  | 15             |
| 1   | A     | 26  | HIS  | 13             |
| 1   | A     | 31  | GLU  | 12             |
| 1   | A     | 33  | THR  | 12             |
| 1   | A     | 70  | MET  | 12             |
| 1   | A     | 80  | ARG  | 9              |
| 1   | A     | 36  | ARG  | 8              |
| 1   | A     | 60  | ASN  | 8              |
| 1   | A     | 4   | SER  | 8              |
| 1   | A     | 48  | LEU  | 7              |
| 1   | A     | 46  | CYS  | 7              |
| 1   | A     | 8   | VAL  | 5              |
| 1   | A     | 72  | ASN  | 4              |
| 1   | A     | 64  | GLU  | 4              |
| 1   | A     | 29  | GLU  | 3              |
| 1   | A     | 79  | GLN  | 2              |
| 1   | A     | 17  | VAL  | 2              |
| 1   | A     | 76  | ASP  | 1              |
| 1   | A     | 88  | GLU  | 1              |
| 1   | A     | 92  | GLN  | 1              |
| 1   | A     | 6   | SER  | 1              |
| 1   | A     | 57  | MET  | 1              |
| 1   | A     | 56  | LEU  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 9   | ARG  | 1              |
| 1   | A     | 22  | LYS  | 1              |
| 1   | A     | 38  | PHE  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 81% for the well-defined parts and 80% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 7.1.1 Bookkeeping

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                  | 1041 |
| Number of shifts mapped to atoms        | 1041 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 6    |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 94       | $-0.26 \pm 0.16$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 91       | $-0.10 \pm 0.18$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 85       | $0.09 \pm 0.10$                 | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 86       | $-0.21 \pm 0.29$                | None needed ( $< 0.5$ ppm) |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 81%, i.e. 973 atoms were assigned a chemical shift out of a possible 1196. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 410/419 (98%) | 165/168 (98%) | 165/170 (97%)   | 80/81 (99%)     |
| Sidechain | 544/658 (83%) | 370/429 (86%) | 174/202 (86%)   | 0/27 (0%)       |

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|          | Total          | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|----------------|----------------|-----------------|-----------------|
| Aromatic | 19/119 (16%)   | 17/59 (29%)    | 0/44 (0%)       | 2/16 (12%)      |
| Overall  | 973/1196 (81%) | 552/656 (84%)  | 339/416 (81%)   | 82/124 (66%)    |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 1041 atoms were assigned a chemical shift out of a possible 1307. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 446/475 (94%)   | 181/191 (95%)  | 179/192 (93%)   | 86/92 (93%)     |
| Sidechain | 575/703 (82%)   | 391/456 (86%)  | 184/219 (84%)   | 0/28 (0%)       |
| Aromatic  | 20/129 (16%)    | 18/64 (28%)    | 0/49 (0%)       | 2/16 (12%)      |
| Overall   | 1041/1307 (80%) | 590/711 (83%)  | 363/460 (79%)   | 88/136 (65%)    |

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

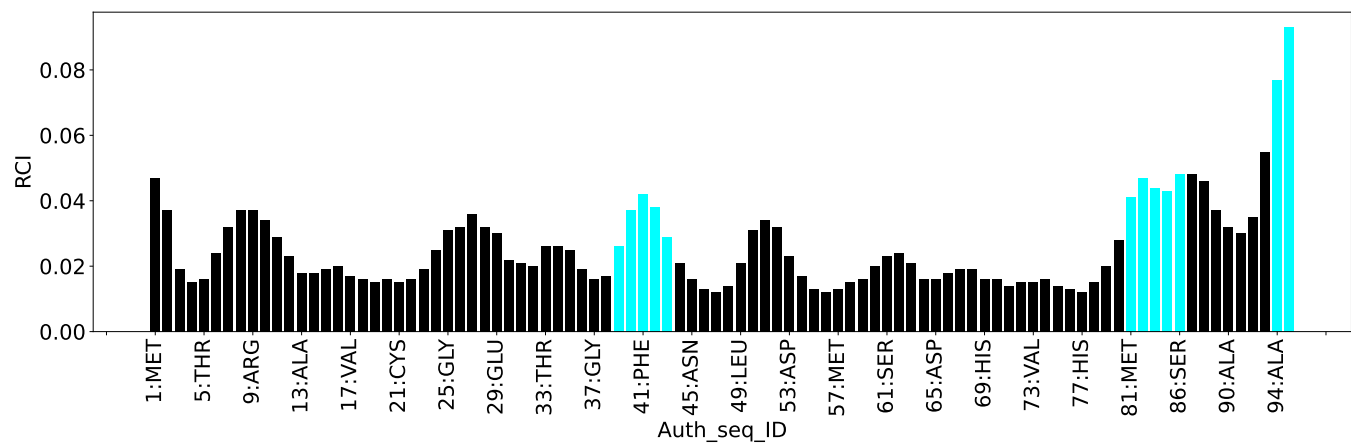
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 71  | GLN  | HG3  | -0.21      | 0.91 – 3.68         | -9.1    |
| 1       | A     | 6   | SER  | HB3  | 2.04       | 2.49 – 5.20         | -6.7    |
| 1       | A     | 6   | SER  | HB2  | 2.27       | 2.61 – 5.13         | -6.4    |
| 1       | A     | 39  | ILE  | HG21 | -0.57      | -0.56 – 2.11        | -5.0    |
| 1       | A     | 39  | ILE  | HG22 | -0.57      | -0.56 – 2.11        | -5.0    |
| 1       | A     | 39  | ILE  | HG23 | -0.57      | -0.56 – 2.11        | -5.0    |

#### 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                                | 1404  |
| Intra-residue ( $ i-j =0$ )                              | 393   |
| Sequential ( $ i-j =1$ )                                 | 373   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 257   |
| Long range ( $ i-j \geq 5$ )                             | 381   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 144   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 13.1  |
| Number of long range restraints per residue <sup>1</sup> | 3.2   |

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

### 8.2 Residual restraint violations

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

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

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

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|----------------------------------------|---------|
| 0.1-0.2 (Small)  | 42.1                                   | 0.2     |
| 0.2-0.5 (Medium) | 1.8                                    | 0.48    |
| >0.5 (Large)     | 0.3                                    | 0.9     |

### 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)   | 11.2                                   | 3.87    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis

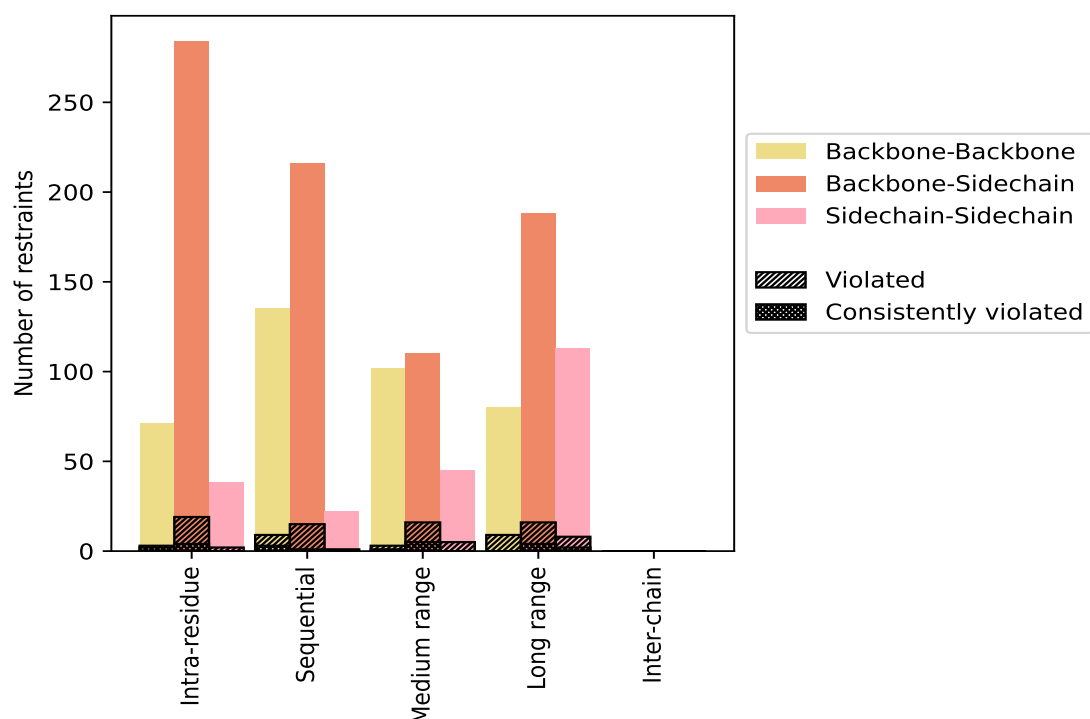
### 9.1 Summary of distance violations

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

| Restrains type                                             | Count                | % <sup>1</sup>        | Violated <sup>3</sup> |                     |                     | Consistently Violated <sup>4</sup> |                     |                     |
|------------------------------------------------------------|----------------------|-----------------------|-----------------------|---------------------|---------------------|------------------------------------|---------------------|---------------------|
|                                                            |                      |                       | Count                 | % <sup>2</sup>      | % <sup>1</sup>      | Count                              | % <sup>2</sup>      | % <sup>1</sup>      |
| <a href="#">Intra-residue ( i-j =0)</a>                    | <a href="#">393</a>  | <a href="#">28.0</a>  | <a href="#">24</a>    | <a href="#">6.1</a> | <a href="#">1.7</a> | <a href="#">6</a>                  | <a href="#">1.5</a> | <a href="#">0.4</a> |
| Backbone-Backbone                                          | 71                   | 5.1                   | 3                     | 4.2                 | 0.2                 | 2                                  | 2.8                 | 0.1                 |
| Backbone-Sidechain                                         | 284                  | 20.2                  | 19                    | 6.7                 | 1.4                 | 4                                  | 1.4                 | 0.3                 |
| Sidechain-Sidechain                                        | 38                   | 2.7                   | 2                     | 5.3                 | 0.1                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">373</a>  | <a href="#">26.6</a>  | <a href="#">25</a>    | <a href="#">6.7</a> | <a href="#">1.8</a> | <a href="#">4</a>                  | <a href="#">1.1</a> | <a href="#">0.3</a> |
| Backbone-Backbone                                          | 135                  | 9.6                   | 9                     | 6.7                 | 0.6                 | 3                                  | 2.2                 | 0.2                 |
| Backbone-Sidechain                                         | 216                  | 15.4                  | 15                    | 6.9                 | 1.1                 | 1                                  | 0.5                 | 0.1                 |
| Sidechain-Sidechain                                        | 22                   | 1.6                   | 1                     | 4.5                 | 0.1                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">257</a>  | <a href="#">18.3</a>  | <a href="#">24</a>    | <a href="#">9.3</a> | <a href="#">1.7</a> | <a href="#">6</a>                  | <a href="#">2.3</a> | <a href="#">0.4</a> |
| Backbone-Backbone                                          | 102                  | 7.3                   | 3                     | 2.9                 | 0.2                 | 1                                  | 1.0                 | 0.1                 |
| Backbone-Sidechain                                         | 110                  | 7.8                   | 16                    | 14.5                | 1.1                 | 5                                  | 4.5                 | 0.4                 |
| Sidechain-Sidechain                                        | 45                   | 3.2                   | 5                     | 11.1                | 0.4                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">381</a>  | <a href="#">27.1</a>  | <a href="#">33</a>    | <a href="#">8.7</a> | <a href="#">2.4</a> | <a href="#">6</a>                  | <a href="#">1.6</a> | <a href="#">0.4</a> |
| Backbone-Backbone                                          | 80                   | 5.7                   | 9                     | 11.2                | 0.6                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 188                  | 13.4                  | 16                    | 8.5                 | 1.1                 | 4                                  | 2.1                 | 0.3                 |
| Sidechain-Sidechain                                        | 113                  | 8.0                   | 8                     | 7.1                 | 0.6                 | 2                                  | 1.8                 | 0.1                 |
| <a href="#">Inter-chain</a>                                | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a> | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 0                    | 0.0                   | 0                     | 0.0                 | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 0                    | 0.0                   | 0                     | 0.0                 | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 0                    | 0.0                   | 0                     | 0.0                 | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Hydrogen bond</a>                              | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a> | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| <a href="#">Disulfide bond</a>                             | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a> | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| <a href="#">Total</a>                                      | <a href="#">1404</a> | <a href="#">100.0</a> | <a href="#">106</a>   | <a href="#">7.5</a> | <a href="#">7.5</a> | <a href="#">22</a>                 | <a href="#">1.6</a> | <a href="#">1.6</a> |
| Backbone-Backbone                                          | 388                  | 27.6                  | 24                    | 6.2                 | 1.7                 | 6                                  | 1.5                 | 0.4                 |
| Backbone-Sidechain                                         | 798                  | 56.8                  | 66                    | 8.3                 | 4.7                 | 14                                 | 1.8                 | 1.0                 |
| Sidechain-Sidechain                                        | 218                  | 15.5                  | 16                    | 7.3                 | 1.1                 | 2                                  | 0.9                 | 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 disulfied bonds are counted in their appropriate category on the x-axis

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 11                   | 13              | 14              | 18              | 0               | 56    | 0.13     | 0.47    | 0.05                | 0.12       |
| 2        | 9                    | 10              | 13              | 15              | 0               | 47    | 0.14     | 0.35    | 0.05                | 0.13       |
| 3        | 11                   | 12              | 11              | 13              | 0               | 47    | 0.14     | 0.43    | 0.05                | 0.12       |
| 4        | 13                   | 14              | 10              | 15              | 0               | 52    | 0.13     | 0.38    | 0.04                | 0.12       |
| 5        | 7                    | 14              | 15              | 17              | 0               | 53    | 0.15     | 0.89    | 0.12                | 0.12       |
| 6        | 10                   | 14              | 11              | 15              | 0               | 50    | 0.16     | 0.55    | 0.1                 | 0.13       |
| 7        | 10                   | 11              | 11              | 18              | 0               | 50    | 0.14     | 0.41    | 0.05                | 0.13       |
| 8        | 13                   | 11              | 13              | 14              | 0               | 51    | 0.14     | 0.34    | 0.04                | 0.13       |
| 9        | 12                   | 13              | 13              | 18              | 0               | 56    | 0.13     | 0.42    | 0.05                | 0.12       |
| 10       | 10                   | 9               | 11              | 13              | 0               | 43    | 0.13     | 0.48    | 0.06                | 0.12       |

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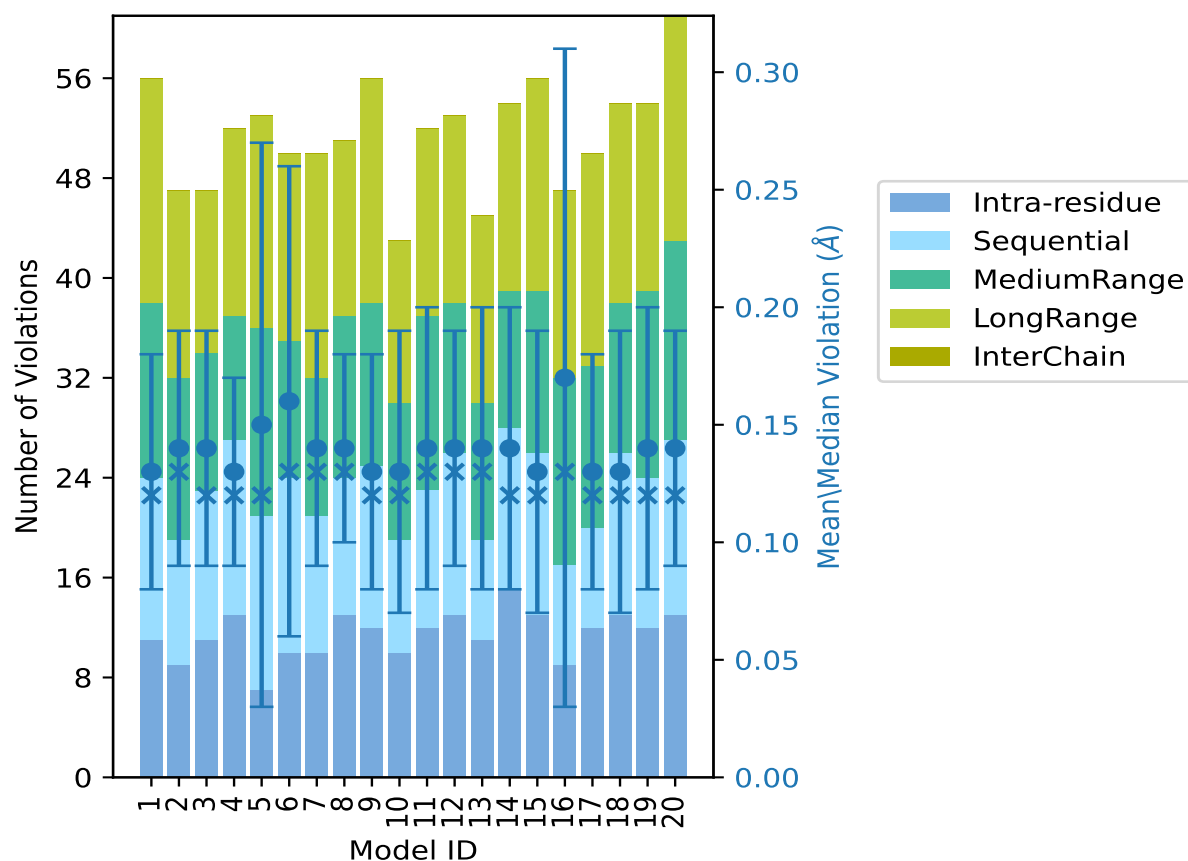
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 12                   | 11              | 14              | 15              | 0               | 52    | 0.14     | 0.46    | 0.06                | 0.13       |
| 12       | 13                   | 13              | 12              | 15              | 0               | 53    | 0.14     | 0.43    | 0.05                | 0.13       |
| 13       | 11                   | 8               | 11              | 15              | 0               | 45    | 0.14     | 0.54    | 0.06                | 0.13       |
| 14       | 15                   | 13              | 11              | 15              | 0               | 54    | 0.14     | 0.46    | 0.06                | 0.12       |
| 15       | 13                   | 13              | 13              | 17              | 0               | 56    | 0.13     | 0.46    | 0.06                | 0.12       |
| 16       | 9                    | 8               | 15              | 15              | 0               | 47    | 0.17     | 0.9     | 0.14                | 0.13       |
| 17       | 12                   | 8               | 13              | 17              | 0               | 50    | 0.13     | 0.41    | 0.05                | 0.12       |
| 18       | 13                   | 13              | 12              | 16              | 0               | 54    | 0.13     | 0.46    | 0.06                | 0.12       |
| 19       | 12                   | 12              | 15              | 15              | 0               | 54    | 0.14     | 0.46    | 0.06                | 0.12       |
| 20       | 13                   | 14              | 16              | 18              | 0               | 61    | 0.14     | 0.43    | 0.05                | 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

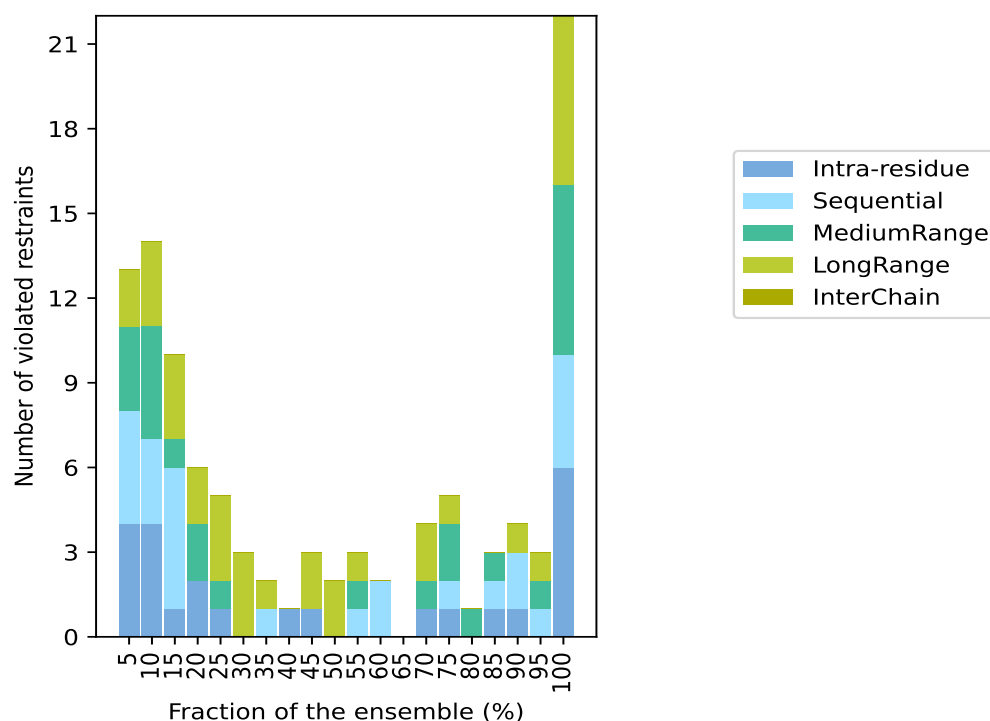
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1298(IR:369, SQ:348, MR:233, LR:348, IC:0) restraints are 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>       | %     |
| 4                             | 4               | 3               | 2               | 0               | 13    | 1                        | 5.0   |
| 4                             | 3               | 4               | 3               | 0               | 14    | 2                        | 10.0  |
| 1                             | 5               | 1               | 3               | 0               | 10    | 3                        | 15.0  |
| 2                             | 0               | 2               | 2               | 0               | 6     | 4                        | 20.0  |
| 1                             | 0               | 1               | 3               | 0               | 5     | 5                        | 25.0  |
| 0                             | 0               | 0               | 3               | 0               | 3     | 6                        | 30.0  |
| 0                             | 1               | 0               | 1               | 0               | 2     | 7                        | 35.0  |
| 1                             | 0               | 0               | 0               | 0               | 1     | 8                        | 40.0  |
| 1                             | 0               | 0               | 2               | 0               | 3     | 9                        | 45.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 10                       | 50.0  |
| 0                             | 1               | 1               | 1               | 0               | 3     | 11                       | 55.0  |
| 0                             | 2               | 0               | 0               | 0               | 2     | 12                       | 60.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 13                       | 65.0  |
| 1                             | 0               | 1               | 2               | 0               | 4     | 14                       | 70.0  |
| 1                             | 1               | 2               | 1               | 0               | 5     | 15                       | 75.0  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 16                       | 80.0  |
| 1                             | 1               | 1               | 0               | 0               | 3     | 17                       | 85.0  |
| 1                             | 2               | 0               | 1               | 0               | 4     | 18                       | 90.0  |
| 0                             | 1               | 1               | 1               | 0               | 3     | 19                       | 95.0  |
| 6                             | 4               | 6               | 6               | 0               | 22    | 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

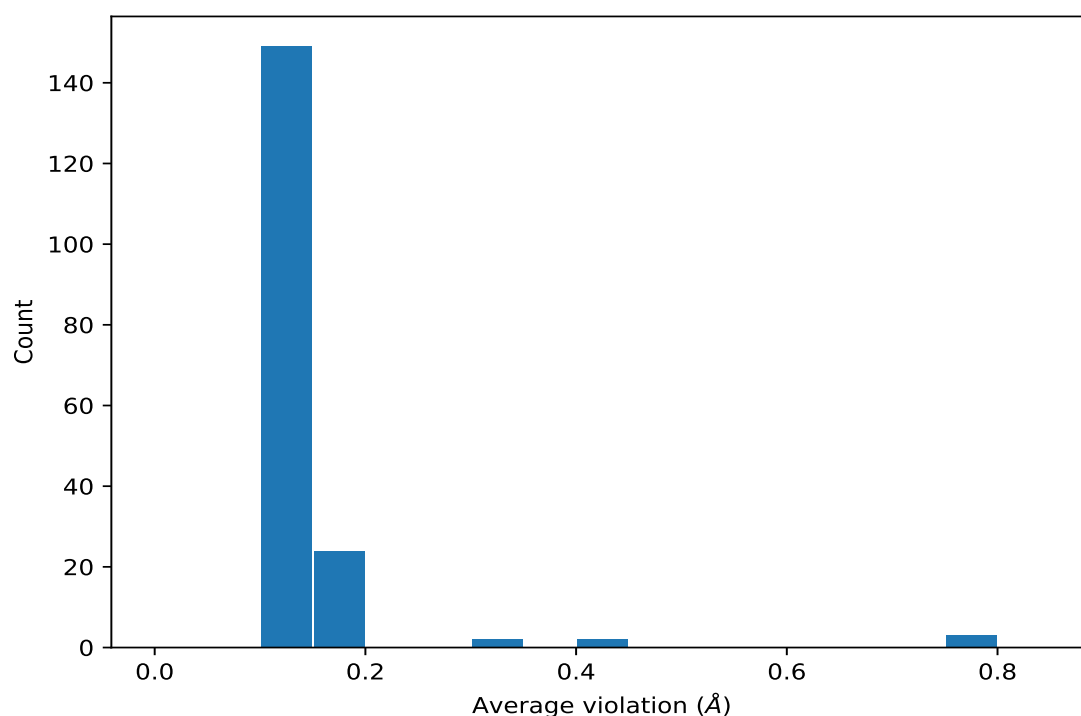
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|----------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,745)  | 1:4:A:SER:HB2   | 1:94:A:ALA:HB1 | 20                  | 0.44     | 0.04                | 0.44       |
| (1,745)  | 1:4:A:SER:HB3   | 1:94:A:ALA:HB1 | 20                  | 0.44     | 0.04                | 0.44       |
| (1,60)   | 1:13:A:ALA:HB1  | 1:51:A:HIS:H   | 20                  | 0.19     | 0.01                | 0.19       |
| (1,60)   | 1:13:A:ALA:HB2  | 1:51:A:HIS:H   | 20                  | 0.19     | 0.01                | 0.19       |
| (1,60)   | 1:13:A:ALA:HB3  | 1:51:A:HIS:H   | 20                  | 0.19     | 0.01                | 0.19       |
| (1,30)   | 1:11:A:GLU:HG2  | 1:13:A:ALA:H   | 20                  | 0.16     | 0.01                | 0.16       |
| (1,30)   | 1:11:A:GLU:HG3  | 1:13:A:ALA:H   | 20                  | 0.16     | 0.01                | 0.16       |
| (1,948)  | 1:64:A:GLU:HA   | 1:64:A:GLU:H   | 20                  | 0.16     | 0.01                | 0.16       |
| (1,958)  | 1:64:A:GLU:HB2  | 1:64:A:GLU:H   | 20                  | 0.16     | 0.0                 | 0.16       |
| (1,1001) | 1:67:A:LEU:HB3  | 1:67:A:LEU:H   | 20                  | 0.16     | 0.01                | 0.16       |
| (1,1015) | 1:68:A:ALA:HA   | 1:71:A:GLN:HB2 | 20                  | 0.15     | 0.01                | 0.15       |
| (1,9)    | 1:10:A:THR:HG21 | 1:53:A:ASP:HA  | 20                  | 0.14     | 0.01                | 0.14       |
| (1,9)    | 1:10:A:THR:HG22 | 1:53:A:ASP:HA  | 20                  | 0.14     | 0.01                | 0.14       |
| (1,9)    | 1:10:A:THR:HG23 | 1:53:A:ASP:HA  | 20                  | 0.14     | 0.01                | 0.14       |
| (1,589)  | 1:3:A:ARG:HB2   | 1:3:A:ARG:H    | 20                  | 0.14     | 0.01                | 0.14       |
| (1,589)  | 1:3:A:ARG:HB3   | 1:3:A:ARG:H    | 20                  | 0.14     | 0.01                | 0.14       |

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| Key      | Atom-1          | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,922)  | 1:62:A:PRO:HB3  | 1:63:A:ASP:H   | 20                  | 0.14     | 0.01                | 0.14       |
| (1,878)  | 1:5:A:THR:HA    | 1:5:A:THR:HG21 | 20                  | 0.13     | 0.0                 | 0.13       |
| (1,878)  | 1:5:A:THR:HA    | 1:5:A:THR:HG22 | 20                  | 0.13     | 0.0                 | 0.13       |
| (1,878)  | 1:5:A:THR:HA    | 1:5:A:THR:HG23 | 20                  | 0.13     | 0.0                 | 0.13       |
| (1,726)  | 1:49:A:LEU:H    | 1:57:A:MET:HG2 | 20                  | 0.13     | 0.01                | 0.14       |
| (1,914)  | 1:61:A:SER:HB2  | 1:67:A:LEU:HA  | 20                  | 0.13     | 0.02                | 0.13       |
| (1,914)  | 1:61:A:SER:HB3  | 1:67:A:LEU:HA  | 20                  | 0.13     | 0.02                | 0.13       |
| (1,744)  | 1:4:A:SER:HB2   | 1:93:A:PRO:HB2 | 20                  | 0.13     | 0.01                | 0.13       |
| (1,744)  | 1:4:A:SER:HB3   | 1:93:A:PRO:HB2 | 20                  | 0.13     | 0.01                | 0.13       |
| (1,942)  | 1:63:A:ASP:H    | 1:67:A:LEU:HB3 | 20                  | 0.13     | 0.01                | 0.13       |
| (1,454)  | 1:33:A:THR:HA   | 1:33:A:THR:H   | 20                  | 0.13     | 0.0                 | 0.13       |
| (1,800)  | 1:54:A:HIS:HA   | 1:55:A:VAL:H   | 20                  | 0.12     | 0.01                | 0.12       |
| (1,832)  | 1:57:A:MET:HA   | 1:58:A:ILE:H   | 20                  | 0.12     | 0.01                | 0.12       |
| (1,992)  | 1:66:A:SER:H    | 1:67:A:LEU:H   | 20                  | 0.12     | 0.01                | 0.12       |
| (1,1145) | 1:74:A:VAL:HB   | 1:76:A:ASP:H   | 20                  | 0.12     | 0.01                | 0.12       |
| (1,954)  | 1:64:A:GLU:HA   | 1:67:A:LEU:HG  | 20                  | 0.12     | 0.01                | 0.12       |
| (1,938)  | 1:63:A:ASP:H    | 1:66:A:SER:HA  | 20                  | 0.12     | 0.01                | 0.12       |
| (1,1328) | 1:89:A:ILE:HG21 | 1:91:A:TRP:H   | 19                  | 0.13     | 0.01                | 0.13       |
| (1,1328) | 1:89:A:ILE:HG22 | 1:91:A:TRP:H   | 19                  | 0.13     | 0.01                | 0.13       |
| (1,1328) | 1:89:A:ILE:HG23 | 1:91:A:TRP:H   | 19                  | 0.13     | 0.01                | 0.13       |
| (1,521)  | 1:38:A:PHE:HA   | 1:46:A:CYS:H   | 19                  | 0.13     | 0.02                | 0.13       |
| (1,773)  | 1:51:A:HIS:H    | 1:52:A:PRO:HD3 | 19                  | 0.11     | 0.01                | 0.11       |
| (1,120)  | 1:16:A:TYR:HA   | 1:16:A:TYR:HD1 | 18                  | 0.15     | 0.01                | 0.15       |
| (1,120)  | 1:16:A:TYR:HA   | 1:16:A:TYR:HD2 | 18                  | 0.15     | 0.01                | 0.15       |
| (1,472)  | 1:34:A:PRO:HB3  | 1:35:A:GLU:H   | 18                  | 0.11     | 0.01                | 0.12       |
| (1,601)  | 1:3:A:ARG:HG2   | 1:61:A:SER:H   | 18                  | 0.11     | 0.01                | 0.11       |
| (1,774)  | 1:51:A:HIS:H    | 1:52:A:PRO:HD2 | 18                  | 0.11     | 0.0                 | 0.11       |
| (1,1263) | 1:7:A:HIS:HD2   | 1:9:A:ARG:HG3  | 17                  | 0.33     | 0.12                | 0.32       |
| (1,1263) | 1:7:A:HIS:HD1   | 1:9:A:ARG:HG3  | 17                  | 0.33     | 0.12                | 0.32       |
| (1,1309) | 1:87:A:LEU:HB2  | 1:87:A:LEU:H   | 17                  | 0.13     | 0.02                | 0.12       |
| (1,29)   | 1:11:A:GLU:HG2  | 1:12:A:SER:H   | 17                  | 0.1      | 0.0                 | 0.1        |
| (1,29)   | 1:11:A:GLU:HG3  | 1:12:A:SER:H   | 17                  | 0.1      | 0.0                 | 0.1        |
| (1,5)    | 1:10:A:THR:HG21 | 1:13:A:ALA:HA  | 16                  | 0.12     | 0.01                | 0.12       |
| (1,5)    | 1:10:A:THR:HG22 | 1:13:A:ALA:HA  | 16                  | 0.12     | 0.01                | 0.12       |
| (1,5)    | 1:10:A:THR:HG23 | 1:13:A:ALA:HA  | 16                  | 0.12     | 0.01                | 0.12       |
| (1,194)  | 1:19:A:ARG:H    | 1:20:A:LEU:HG  | 15                  | 0.15     | 0.02                | 0.14       |
| (1,96)   | 1:15:A:ARG:HA   | 1:19:A:ARG:H   | 15                  | 0.13     | 0.02                | 0.12       |
| (1,56)   | 1:13:A:ALA:HB1  | 1:16:A:TYR:HD1 | 15                  | 0.12     | 0.01                | 0.11       |
| (1,56)   | 1:13:A:ALA:HB1  | 1:16:A:TYR:HD2 | 15                  | 0.12     | 0.01                | 0.11       |
| (1,56)   | 1:13:A:ALA:HB2  | 1:16:A:TYR:HD1 | 15                  | 0.12     | 0.01                | 0.11       |
| (1,56)   | 1:13:A:ALA:HB2  | 1:16:A:TYR:HD2 | 15                  | 0.12     | 0.01                | 0.11       |
| (1,56)   | 1:13:A:ALA:HB3  | 1:16:A:TYR:HD1 | 15                  | 0.12     | 0.01                | 0.11       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,56)   | 1:13:A:ALA:HB3  | 1:16:A:TYR:HD2  | 15                  | 0.12     | 0.01                | 0.11       |
| (1,1342) | 1:90:A:ALA:HB1  | 1:90:A:ALA:H    | 15                  | 0.11     | 0.01                | 0.11       |
| (1,1342) | 1:90:A:ALA:HB2  | 1:90:A:ALA:H    | 15                  | 0.11     | 0.01                | 0.11       |
| (1,1342) | 1:90:A:ALA:HB3  | 1:90:A:ALA:H    | 15                  | 0.11     | 0.01                | 0.11       |
| (1,51)   | 1:13:A:ALA:HA   | 1:51:A:HIS:H    | 15                  | 0.1      | 0.0                 | 0.1        |
| (1,704)  | 1:48:A:LEU:HB2  | 1:48:A:LEU:H    | 14                  | 0.13     | 0.01                | 0.13       |
| (1,704)  | 1:48:A:LEU:HB3  | 1:48:A:LEU:H    | 14                  | 0.13     | 0.01                | 0.13       |
| (1,673)  | 1:45:A:ASN:H    | 1:70:A:MET:HB3  | 14                  | 0.13     | 0.02                | 0.14       |
| (1,739)  | 1:4:A:SER:HB2   | 1:59:A:LEU:HB2  | 14                  | 0.11     | 0.01                | 0.11       |
| (1,739)  | 1:4:A:SER:HB2   | 1:59:A:LEU:HB3  | 14                  | 0.11     | 0.01                | 0.11       |
| (1,739)  | 1:4:A:SER:HB3   | 1:59:A:LEU:HB2  | 14                  | 0.11     | 0.01                | 0.11       |
| (1,739)  | 1:4:A:SER:HB3   | 1:59:A:LEU:HB3  | 14                  | 0.11     | 0.01                | 0.11       |
| (1,1308) | 1:87:A:LEU:HB3  | 1:89:A:ILE:HA   | 14                  | 0.11     | 0.0                 | 0.11       |
| (1,511)  | 1:37:A:GLY:HA2  | 1:38:A:PHE:H    | 12                  | 0.16     | 0.01                | 0.16       |
| (1,151)  | 1:17:A:VAL:HG11 | 1:18:A:ASN:H    | 12                  | 0.12     | 0.02                | 0.12       |
| (1,151)  | 1:17:A:VAL:HG12 | 1:18:A:ASN:H    | 12                  | 0.12     | 0.02                | 0.12       |
| (1,151)  | 1:17:A:VAL:HG13 | 1:18:A:ASN:H    | 12                  | 0.12     | 0.02                | 0.12       |
| (1,176)  | 1:18:A:ASN:H    | 1:19:A:ARG:H    | 11                  | 0.11     | 0.01                | 0.11       |
| (1,1063) | 1:6:A:SER:H     | 1:58:A:ILE:HG21 | 11                  | 0.11     | 0.0                 | 0.11       |
| (1,1063) | 1:6:A:SER:H     | 1:58:A:ILE:HG22 | 11                  | 0.11     | 0.0                 | 0.11       |
| (1,1063) | 1:6:A:SER:H     | 1:58:A:ILE:HG23 | 11                  | 0.11     | 0.0                 | 0.11       |
| (1,964)  | 1:64:A:GLU:HG2  | 1:67:A:LEU:HG   | 11                  | 0.1      | 0.0                 | 0.1        |
| (1,964)  | 1:64:A:GLU:HG3  | 1:67:A:LEU:HG   | 11                  | 0.1      | 0.0                 | 0.1        |
| (1,160)  | 1:17:A:VAL:HG21 | 1:36:A:ARG:H    | 10                  | 0.14     | 0.02                | 0.15       |
| (1,160)  | 1:17:A:VAL:HG22 | 1:36:A:ARG:H    | 10                  | 0.14     | 0.02                | 0.15       |
| (1,160)  | 1:17:A:VAL:HG23 | 1:36:A:ARG:H    | 10                  | 0.14     | 0.02                | 0.15       |
| (1,295)  | 1:24:A:TRP:H    | 1:39:A:ILE:HG21 | 10                  | 0.11     | 0.01                | 0.11       |
| (1,295)  | 1:24:A:TRP:H    | 1:39:A:ILE:HG22 | 10                  | 0.11     | 0.01                | 0.11       |
| (1,295)  | 1:24:A:TRP:H    | 1:39:A:ILE:HG23 | 10                  | 0.11     | 0.01                | 0.11       |
| (1,724)  | 1:49:A:LEU:H    | 1:57:A:MET:HA   | 9                   | 0.11     | 0.01                | 0.11       |
| (1,738)  | 1:4:A:SER:HB2   | 1:94:A:ALA:H    | 9                   | 0.11     | 0.01                | 0.11       |
| (1,398)  | 1:30:A:VAL:HA   | 1:30:A:VAL:HG11 | 9                   | 0.1      | 0.01                | 0.1        |
| (1,398)  | 1:30:A:VAL:HA   | 1:30:A:VAL:HG12 | 9                   | 0.1      | 0.01                | 0.1        |
| (1,398)  | 1:30:A:VAL:HA   | 1:30:A:VAL:HG13 | 9                   | 0.1      | 0.01                | 0.1        |
| (1,54)   | 1:13:A:ALA:HB1  | 1:13:A:ALA:H    | 8                   | 0.11     | 0.0                 | 0.11       |
| (1,54)   | 1:13:A:ALA:HB2  | 1:13:A:ALA:H    | 8                   | 0.11     | 0.0                 | 0.11       |
| (1,54)   | 1:13:A:ALA:HB3  | 1:13:A:ALA:H    | 8                   | 0.11     | 0.0                 | 0.11       |
| (1,116)  | 1:15:A:ARG:HG2  | 1:16:A:TYR:H    | 7                   | 0.12     | 0.01                | 0.12       |
| (1,116)  | 1:15:A:ARG:HG3  | 1:16:A:TYR:H    | 7                   | 0.12     | 0.01                | 0.12       |
| (1,493)  | 1:36:A:ARG:HA   | 1:49:A:LEU:HA   | 7                   | 0.12     | 0.02                | 0.11       |
| (1,113)  | 1:15:A:ARG:HD2  | 1:20:A:LEU:H    | 6                   | 0.12     | 0.02                | 0.12       |
| (1,113)  | 1:15:A:ARG:HD3  | 1:20:A:LEU:H    | 6                   | 0.12     | 0.02                | 0.12       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,394)  | 1:2:A:PHE:H     | 1:62:A:PRO:HD2  | 6                   | 0.11     | 0.01                | 0.11       |
| (1,394)  | 1:2:A:PHE:H     | 1:62:A:PRO:HD3  | 6                   | 0.11     | 0.01                | 0.11       |
| (1,85)   | 1:14:A:ALA:HB1  | 1:50:A:ALA:HA   | 6                   | 0.11     | 0.01                | 0.11       |
| (1,85)   | 1:14:A:ALA:HB2  | 1:50:A:ALA:HA   | 6                   | 0.11     | 0.01                | 0.11       |
| (1,85)   | 1:14:A:ALA:HB3  | 1:50:A:ALA:HA   | 6                   | 0.11     | 0.01                | 0.11       |
| (1,808)  | 1:54:A:HIS:HD1  | 1:56:A:LEU:HD12 | 5                   | 0.18     | 0.05                | 0.15       |
| (1,808)  | 1:54:A:HIS:HD1  | 1:56:A:LEU:HD11 | 5                   | 0.18     | 0.05                | 0.15       |
| (1,808)  | 1:54:A:HIS:HD1  | 1:56:A:LEU:HD13 | 5                   | 0.18     | 0.05                | 0.15       |
| (1,651)  | 1:44:A:SER:HB3  | 1:61:A:SER:HA   | 5                   | 0.14     | 0.04                | 0.13       |
| (1,372)  | 1:29:A:GLU:H    | 1:41:A:PHE:HA   | 5                   | 0.11     | 0.02                | 0.1        |
| (1,437)  | 1:32:A:LEU:HB3  | 1:32:A:LEU:H    | 5                   | 0.11     | 0.01                | 0.11       |
| (1,283)  | 1:23:A:HIS:H    | 1:30:A:VAL:HG21 | 5                   | 0.11     | 0.0                 | 0.11       |
| (1,283)  | 1:23:A:HIS:H    | 1:30:A:VAL:HG22 | 5                   | 0.11     | 0.0                 | 0.11       |
| (1,283)  | 1:23:A:HIS:H    | 1:30:A:VAL:HG23 | 5                   | 0.11     | 0.0                 | 0.11       |
| (1,279)  | 1:23:A:HIS:HD2  | 1:25:A:GLY:H    | 4                   | 0.18     | 0.02                | 0.17       |
| (1,279)  | 1:23:A:HIS:HD1  | 1:25:A:GLY:H    | 4                   | 0.18     | 0.02                | 0.17       |
| (1,1127) | 1:73:A:VAL:HG12 | 1:77:A:HIS:HD2  | 4                   | 0.17     | 0.08                | 0.16       |
| (1,1127) | 1:73:A:VAL:HG12 | 1:77:A:HIS:HD1  | 4                   | 0.17     | 0.08                | 0.16       |
| (1,1315) | 1:87:A:LEU:HG   | 1:87:A:LEU:H    | 4                   | 0.11     | 0.01                | 0.11       |
| (1,571)  | 1:39:A:ILE:H    | 1:46:A:CYS:H    | 4                   | 0.11     | 0.01                | 0.11       |
| (1,1386) | 1:9:A:ARG:HA    | 1:54:A:HIS:HA   | 4                   | 0.1      | 0.0                 | 0.1        |
| (1,71)   | 1:14:A:ALA:HA   | 1:14:A:ALA:H    | 4                   | 0.1      | 0.0                 | 0.1        |
| (1,1261) | 1:7:A:HIS:HD1   | 1:56:A:LEU:HD23 | 3                   | 0.78     | 0.16                | 0.89       |
| (1,1261) | 1:7:A:HIS:HD2   | 1:56:A:LEU:HD22 | 3                   | 0.78     | 0.16                | 0.89       |
| (1,1261) | 1:7:A:HIS:HD1   | 1:56:A:LEU:HD21 | 3                   | 0.78     | 0.16                | 0.89       |
| (1,292)  | 1:24:A:TRP:HB2  | 1:39:A:ILE:HG21 | 3                   | 0.12     | 0.01                | 0.11       |
| (1,292)  | 1:24:A:TRP:HB2  | 1:39:A:ILE:HG22 | 3                   | 0.12     | 0.01                | 0.11       |
| (1,292)  | 1:24:A:TRP:HB2  | 1:39:A:ILE:HG23 | 3                   | 0.12     | 0.01                | 0.11       |
| (1,292)  | 1:24:A:TRP:HB3  | 1:39:A:ILE:HG21 | 3                   | 0.12     | 0.01                | 0.11       |
| (1,292)  | 1:24:A:TRP:HB3  | 1:39:A:ILE:HG22 | 3                   | 0.12     | 0.01                | 0.11       |
| (1,292)  | 1:24:A:TRP:HB3  | 1:39:A:ILE:HG23 | 3                   | 0.12     | 0.01                | 0.11       |
| (1,98)   | 1:15:A:ARG:HB3  | 1:17:A:VAL:H    | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,195)  | 1:19:A:ARG:H    | 1:20:A:LEU:H    | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,969)  | 1:64:A:GLU:H    | 1:65:A:ASP:H    | 3                   | 0.11     | 0.01                | 0.12       |
| (1,134)  | 1:16:A:TYR:H    | 1:17:A:VAL:HB   | 3                   | 0.11     | 0.01                | 0.11       |
| (1,534)  | 1:38:A:PHE:HD1  | 1:45:A:ASN:HB2  | 3                   | 0.11     | 0.01                | 0.11       |
| (1,534)  | 1:38:A:PHE:HD1  | 1:45:A:ASN:HB3  | 3                   | 0.11     | 0.01                | 0.11       |
| (1,534)  | 1:38:A:PHE:HD2  | 1:45:A:ASN:HB2  | 3                   | 0.11     | 0.01                | 0.11       |
| (1,534)  | 1:38:A:PHE:HD2  | 1:45:A:ASN:HB3  | 3                   | 0.11     | 0.01                | 0.11       |
| (1,1276) | 1:80:A:ARG:HG2  | 1:81:A:MET:H    | 3                   | 0.11     | 0.01                | 0.11       |
| (1,284)  | 1:24:A:TRP:HA   | 1:25:A:GLY:H    | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,703)  | 1:48:A:LEU:HB2  | 1:48:A:LEU:HD11 | 3                   | 0.1      | 0.0                 | 0.1        |

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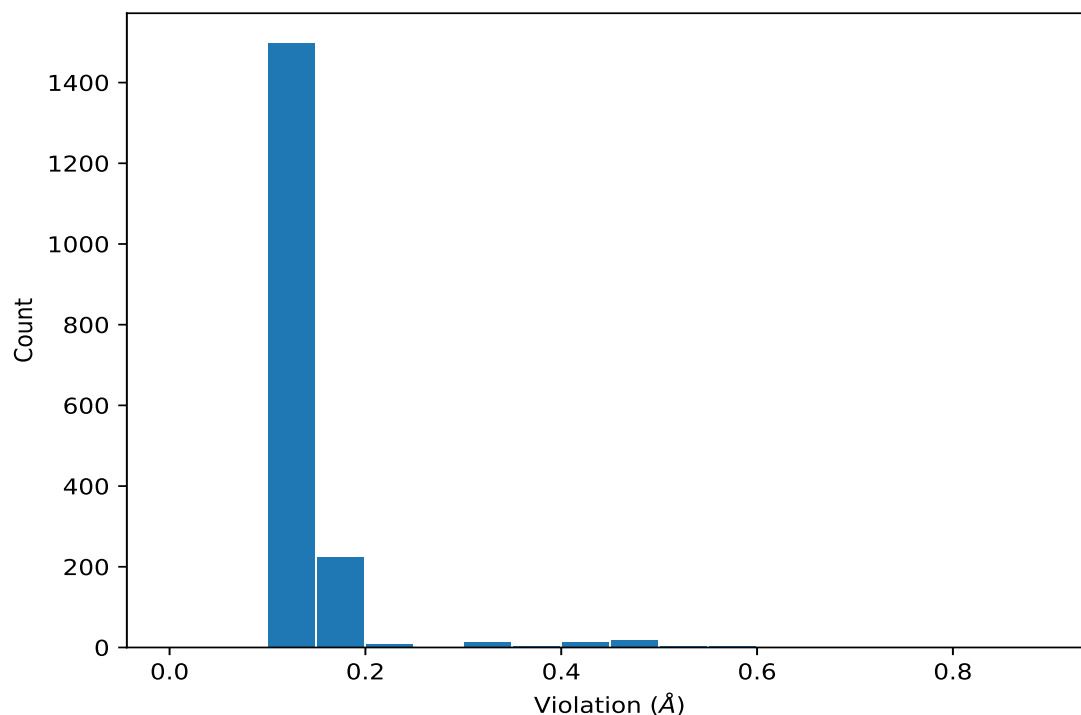
| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,703)  | 1:48:A:LEU:HB2  | 1:48:A:LEU:HD12 | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,703)  | 1:48:A:LEU:HB2  | 1:48:A:LEU:HD13 | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,703)  | 1:48:A:LEU:HB2  | 1:48:A:LEU:HD21 | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,703)  | 1:48:A:LEU:HB2  | 1:48:A:LEU:HD22 | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,703)  | 1:48:A:LEU:HB2  | 1:48:A:LEU:HD23 | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,703)  | 1:48:A:LEU:HB3  | 1:48:A:LEU:HD11 | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,703)  | 1:48:A:LEU:HB3  | 1:48:A:LEU:HD12 | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,703)  | 1:48:A:LEU:HB3  | 1:48:A:LEU:HD13 | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,703)  | 1:48:A:LEU:HB3  | 1:48:A:LEU:HD21 | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,703)  | 1:48:A:LEU:HB3  | 1:48:A:LEU:HD22 | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,703)  | 1:48:A:LEU:HB3  | 1:48:A:LEU:HD23 | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,261)  | 1:22:A:LYS:HE2  | 1:22:A:LYS:HG2  | 2                   | 0.18     | 0.02                | 0.18       |
| (1,261)  | 1:22:A:LYS:HE2  | 1:22:A:LYS:HG3  | 2                   | 0.18     | 0.02                | 0.18       |
| (1,261)  | 1:22:A:LYS:HE3  | 1:22:A:LYS:HG2  | 2                   | 0.18     | 0.02                | 0.18       |
| (1,261)  | 1:22:A:LYS:HE3  | 1:22:A:LYS:HG3  | 2                   | 0.18     | 0.02                | 0.18       |
| (1,791)  | 1:52:A:PRO:HD2  | 1:54:A:HIS:H    | 2                   | 0.14     | 0.03                | 0.14       |
| (1,1138) | 1:74:A:VAL:HA   | 1:77:A:HIS:HB3  | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,1139) | 1:74:A:VAL:HA   | 1:77:A:HIS:HB2  | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,911)  | 1:61:A:SER:HB2  | 1:62:A:PRO:HD2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,911)  | 1:61:A:SER:HB2  | 1:62:A:PRO:HD3  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,911)  | 1:61:A:SER:HB3  | 1:62:A:PRO:HD2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,911)  | 1:61:A:SER:HB3  | 1:62:A:PRO:HD3  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,539)  | 1:38:A:PHE:HD1  | 1:48:A:LEU:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,539)  | 1:38:A:PHE:HD2  | 1:48:A:LEU:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,97)   | 1:15:A:ARG:HB3  | 1:16:A:TYR:H    | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,614)  | 1:40:A:ASP:HB3  | 1:40:A:ASP:H    | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,199)  | 1:1:A:MET:HA    | 1:62:A:PRO:HA   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,335)  | 1:28:A:PHE:HA   | 1:30:A:VAL:HG21 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,335)  | 1:28:A:PHE:HA   | 1:30:A:VAL:HG22 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,335)  | 1:28:A:PHE:HA   | 1:30:A:VAL:HG23 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,191)  | 1:19:A:ARG:HG2  | 1:19:A:ARG:H    | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,191)  | 1:19:A:ARG:HG3  | 1:19:A:ARG:H    | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,542)  | 1:38:A:PHE:HE1  | 1:45:A:ASN:HB2  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,542)  | 1:38:A:PHE:HE1  | 1:45:A:ASN:HB3  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,542)  | 1:38:A:PHE:HE2  | 1:45:A:ASN:HB2  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,542)  | 1:38:A:PHE:HE2  | 1:45:A:ASN:HB3  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,557)  | 1:39:A:ILE:HG13 | 1:39:A:ILE:H    | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,1084) | 1:70:A:MET:H    | 1:71: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) |
|----------|---------------|-----------------|----------|---------------|
| (1,1261) | 1:7:A:HIS:HD1 | 1:56:A:LEU:HD23 | 16       | 0.9           |
| (1,1261) | 1:7:A:HIS:HD2 | 1:56:A:LEU:HD22 | 5        | 0.89          |
| (1,1263) | 1:7:A:HIS:HD2 | 1:9:A:ARG:HG3   | 16       | 0.58          |
| (1,1263) | 1:7:A:HIS:HD2 | 1:9:A:ARG:HG3   | 6        | 0.55          |
| (1,1261) | 1:7:A:HIS:HD1 | 1:56:A:LEU:HD21 | 6        | 0.55          |
| (1,745)  | 1:4:A:SER:HB2 | 1:94:A:ALA:HB1  | 13       | 0.54          |
| (1,745)  | 1:4:A:SER:HB3 | 1:94:A:ALA:HB1  | 13       | 0.54          |
| (1,1263) | 1:7:A:HIS:HD1 | 1:9:A:ARG:HG3   | 5        | 0.53          |
| (1,745)  | 1:4:A:SER:HB2 | 1:94:A:ALA:HB1  | 10       | 0.48          |
| (1,745)  | 1:4:A:SER:HB3 | 1:94:A:ALA:HB1  | 10       | 0.48          |

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| Key      | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|----------|---------------|----------------|----------|---------------|
| (1,745)  | 1:4:A:SER:HB2 | 1:94:A:ALA:HB1 | 1        | 0.47          |
| (1,745)  | 1:4:A:SER:HB3 | 1:94:A:ALA:HB1 | 1        | 0.47          |
| (1,745)  | 1:4:A:SER:HB2 | 1:94:A:ALA:HB1 | 6        | 0.47          |
| (1,745)  | 1:4:A:SER:HB3 | 1:94:A:ALA:HB1 | 6        | 0.47          |
| (1,745)  | 1:4:A:SER:HB2 | 1:94:A:ALA:HB1 | 11       | 0.46          |
| (1,745)  | 1:4:A:SER:HB3 | 1:94:A:ALA:HB1 | 11       | 0.46          |
| (1,745)  | 1:4:A:SER:HB2 | 1:94:A:ALA:HB1 | 14       | 0.46          |
| (1,745)  | 1:4:A:SER:HB3 | 1:94:A:ALA:HB1 | 14       | 0.46          |
| (1,745)  | 1:4:A:SER:HB2 | 1:94:A:ALA:HB1 | 15       | 0.46          |
| (1,745)  | 1:4:A:SER:HB3 | 1:94:A:ALA:HB1 | 15       | 0.46          |
| (1,745)  | 1:4:A:SER:HB2 | 1:94:A:ALA:HB1 | 18       | 0.46          |
| (1,745)  | 1:4:A:SER:HB3 | 1:94:A:ALA:HB1 | 18       | 0.46          |
| (1,745)  | 1:4:A:SER:HB2 | 1:94:A:ALA:HB1 | 19       | 0.46          |
| (1,745)  | 1:4:A:SER:HB3 | 1:94:A:ALA:HB1 | 19       | 0.46          |
| (1,745)  | 1:4:A:SER:HB2 | 1:94:A:ALA:HB1 | 16       | 0.45          |
| (1,745)  | 1:4:A:SER:HB3 | 1:94:A:ALA:HB1 | 16       | 0.45          |
| (1,745)  | 1:4:A:SER:HB2 | 1:94:A:ALA:HB1 | 3        | 0.43          |
| (1,745)  | 1:4:A:SER:HB3 | 1:94:A:ALA:HB1 | 3        | 0.43          |
| (1,745)  | 1:4:A:SER:HB2 | 1:94:A:ALA:HB1 | 12       | 0.43          |
| (1,745)  | 1:4:A:SER:HB3 | 1:94:A:ALA:HB1 | 12       | 0.43          |
| (1,745)  | 1:4:A:SER:HB2 | 1:94:A:ALA:HB1 | 20       | 0.43          |
| (1,745)  | 1:4:A:SER:HB3 | 1:94:A:ALA:HB1 | 20       | 0.43          |
| (1,745)  | 1:4:A:SER:HB2 | 1:94:A:ALA:HB1 | 9        | 0.42          |
| (1,745)  | 1:4:A:SER:HB3 | 1:94:A:ALA:HB1 | 9        | 0.42          |
| (1,745)  | 1:4:A:SER:HB2 | 1:94:A:ALA:HB1 | 5        | 0.41          |
| (1,745)  | 1:4:A:SER:HB3 | 1:94:A:ALA:HB1 | 5        | 0.41          |
| (1,745)  | 1:4:A:SER:HB2 | 1:94:A:ALA:HB1 | 7        | 0.41          |
| (1,745)  | 1:4:A:SER:HB3 | 1:94:A:ALA:HB1 | 7        | 0.41          |
| (1,745)  | 1:4:A:SER:HB2 | 1:94:A:ALA:HB1 | 17       | 0.41          |
| (1,745)  | 1:4:A:SER:HB3 | 1:94:A:ALA:HB1 | 17       | 0.41          |
| (1,745)  | 1:4:A:SER:HB2 | 1:94:A:ALA:HB1 | 4        | 0.38          |
| (1,745)  | 1:4:A:SER:HB3 | 1:94:A:ALA:HB1 | 4        | 0.38          |
| (1,1263) | 1:7:A:HIS:HD1 | 1:9:A:ARG:HG3  | 20       | 0.36          |
| (1,745)  | 1:4:A:SER:HB2 | 1:94:A:ALA:HB1 | 2        | 0.35          |
| (1,745)  | 1:4:A:SER:HB3 | 1:94:A:ALA:HB1 | 2        | 0.35          |
| (1,745)  | 1:4:A:SER:HB2 | 1:94:A:ALA:HB1 | 8        | 0.34          |
| (1,745)  | 1:4:A:SER:HB3 | 1:94:A:ALA:HB1 | 8        | 0.34          |
| (1,1263) | 1:7:A:HIS:HD1 | 1:9:A:ARG:HG3  | 9        | 0.33          |
| (1,1263) | 1:7:A:HIS:HD2 | 1:9:A:ARG:HG3  | 15       | 0.33          |
| (1,1263) | 1:7:A:HIS:HD2 | 1:9:A:ARG:HG3  | 3        | 0.32          |
| (1,1263) | 1:7:A:HIS:HD2 | 1:9:A:ARG:HG3  | 8        | 0.32          |
| (1,1263) | 1:7:A:HIS:HD2 | 1:9:A:ARG:HG3  | 11       | 0.32          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1263) | 1:7:A:HIS:HD2   | 1:9:A:ARG:HG3   | 14       | 0.32          |
| (1,1263) | 1:7:A:HIS:HD2   | 1:9:A:ARG:HG3   | 2        | 0.31          |
| (1,1263) | 1:7:A:HIS:HD2   | 1:9:A:ARG:HG3   | 7        | 0.31          |
| (1,1263) | 1:7:A:HIS:HD2   | 1:9:A:ARG:HG3   | 18       | 0.31          |
| (1,1263) | 1:7:A:HIS:HD2   | 1:9:A:ARG:HG3   | 19       | 0.31          |
| (1,1127) | 1:73:A:VAL:HG12 | 1:77:A:HIS:HD1  | 19       | 0.28          |
| (1,808)  | 1:54:A:HIS:HD1  | 1:56:A:LEU:HD11 | 6        | 0.24          |
| (1,808)  | 1:54:A:HIS:HD1  | 1:56:A:LEU:HD11 | 16       | 0.24          |
| (1,1127) | 1:73:A:VAL:HG12 | 1:77:A:HIS:HD1  | 13       | 0.21          |
| (1,279)  | 1:23:A:HIS:HD1  | 1:25:A:GLY:H    | 17       | 0.21          |
| (1,194)  | 1:19:A:ARG:H    | 1:20:A:LEU:HG   | 20       | 0.2           |
| (1,60)   | 1:13:A:ALA:HB1  | 1:51:A:HIS:H    | 5        | 0.2           |
| (1,60)   | 1:13:A:ALA:HB2  | 1:51:A:HIS:H    | 5        | 0.2           |
| (1,60)   | 1:13:A:ALA:HB3  | 1:51:A:HIS:H    | 5        | 0.2           |
| (1,1263) | 1:7:A:HIS:HD1   | 1:9:A:ARG:HG3   | 12       | 0.19          |
| (1,1001) | 1:67:A:LEU:HB3  | 1:67:A:LEU:H    | 14       | 0.19          |
| (1,1001) | 1:67:A:LEU:HB3  | 1:67:A:LEU:H    | 19       | 0.19          |
| (1,651)  | 1:44:A:SER:HB3  | 1:61:A:SER:HA   | 2        | 0.19          |
| (1,261)  | 1:22:A:LYS:HE2  | 1:22:A:LYS:HG2  | 8        | 0.19          |
| (1,261)  | 1:22:A:LYS:HE2  | 1:22:A:LYS:HG3  | 8        | 0.19          |
| (1,261)  | 1:22:A:LYS:HE3  | 1:22:A:LYS:HG2  | 8        | 0.19          |
| (1,261)  | 1:22:A:LYS:HE3  | 1:22:A:LYS:HG3  | 8        | 0.19          |
| (1,194)  | 1:19:A:ARG:H    | 1:20:A:LEU:HG   | 18       | 0.19          |
| (1,60)   | 1:13:A:ALA:HB1  | 1:51:A:HIS:H    | 1        | 0.19          |
| (1,60)   | 1:13:A:ALA:HB2  | 1:51:A:HIS:H    | 1        | 0.19          |
| (1,60)   | 1:13:A:ALA:HB3  | 1:51:A:HIS:H    | 1        | 0.19          |
| (1,60)   | 1:13:A:ALA:HB1  | 1:51:A:HIS:H    | 2        | 0.19          |
| (1,60)   | 1:13:A:ALA:HB2  | 1:51:A:HIS:H    | 2        | 0.19          |
| (1,60)   | 1:13:A:ALA:HB3  | 1:51:A:HIS:H    | 2        | 0.19          |
| (1,60)   | 1:13:A:ALA:HB1  | 1:51:A:HIS:H    | 3        | 0.19          |
| (1,60)   | 1:13:A:ALA:HB2  | 1:51:A:HIS:H    | 3        | 0.19          |
| (1,60)   | 1:13:A:ALA:HB3  | 1:51:A:HIS:H    | 3        | 0.19          |
| (1,60)   | 1:13:A:ALA:HB1  | 1:51:A:HIS:H    | 4        | 0.19          |
| (1,60)   | 1:13:A:ALA:HB2  | 1:51:A:HIS:H    | 4        | 0.19          |
| (1,60)   | 1:13:A:ALA:HB3  | 1:51:A:HIS:H    | 4        | 0.19          |
| (1,60)   | 1:13:A:ALA:HB1  | 1:51:A:HIS:H    | 7        | 0.19          |
| (1,60)   | 1:13:A:ALA:HB2  | 1:51:A:HIS:H    | 7        | 0.19          |
| (1,60)   | 1:13:A:ALA:HB3  | 1:51:A:HIS:H    | 7        | 0.19          |
| (1,60)   | 1:13:A:ALA:HB1  | 1:51:A:HIS:H    | 8        | 0.19          |
| (1,60)   | 1:13:A:ALA:HB2  | 1:51:A:HIS:H    | 8        | 0.19          |
| (1,60)   | 1:13:A:ALA:HB3  | 1:51:A:HIS:H    | 8        | 0.19          |
| (1,60)   | 1:13:A:ALA:HB1  | 1:51:A:HIS:H    | 9        | 0.19          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,60)   | 1:13:A:ALA:HB2 | 1:51:A:HIS:H   | 9        | 0.19          |
| (1,60)   | 1:13:A:ALA:HB3 | 1:51:A:HIS:H   | 9        | 0.19          |
| (1,60)   | 1:13:A:ALA:HB1 | 1:51:A:HIS:H   | 10       | 0.19          |
| (1,60)   | 1:13:A:ALA:HB2 | 1:51:A:HIS:H   | 10       | 0.19          |
| (1,60)   | 1:13:A:ALA:HB3 | 1:51:A:HIS:H   | 10       | 0.19          |
| (1,60)   | 1:13:A:ALA:HB1 | 1:51:A:HIS:H   | 11       | 0.19          |
| (1,60)   | 1:13:A:ALA:HB2 | 1:51:A:HIS:H   | 11       | 0.19          |
| (1,60)   | 1:13:A:ALA:HB3 | 1:51:A:HIS:H   | 11       | 0.19          |
| (1,60)   | 1:13:A:ALA:HB1 | 1:51:A:HIS:H   | 12       | 0.19          |
| (1,60)   | 1:13:A:ALA:HB2 | 1:51:A:HIS:H   | 12       | 0.19          |
| (1,60)   | 1:13:A:ALA:HB3 | 1:51:A:HIS:H   | 12       | 0.19          |
| (1,60)   | 1:13:A:ALA:HB1 | 1:51:A:HIS:H   | 14       | 0.19          |
| (1,60)   | 1:13:A:ALA:HB2 | 1:51:A:HIS:H   | 14       | 0.19          |
| (1,60)   | 1:13:A:ALA:HB3 | 1:51:A:HIS:H   | 14       | 0.19          |
| (1,60)   | 1:13:A:ALA:HB1 | 1:51:A:HIS:H   | 15       | 0.19          |
| (1,60)   | 1:13:A:ALA:HB2 | 1:51:A:HIS:H   | 15       | 0.19          |
| (1,60)   | 1:13:A:ALA:HB3 | 1:51:A:HIS:H   | 15       | 0.19          |
| (1,60)   | 1:13:A:ALA:HB1 | 1:51:A:HIS:H   | 17       | 0.19          |
| (1,60)   | 1:13:A:ALA:HB2 | 1:51:A:HIS:H   | 17       | 0.19          |
| (1,60)   | 1:13:A:ALA:HB3 | 1:51:A:HIS:H   | 17       | 0.19          |
| (1,60)   | 1:13:A:ALA:HB1 | 1:51:A:HIS:H   | 18       | 0.19          |
| (1,60)   | 1:13:A:ALA:HB2 | 1:51:A:HIS:H   | 18       | 0.19          |
| (1,60)   | 1:13:A:ALA:HB3 | 1:51:A:HIS:H   | 18       | 0.19          |
| (1,60)   | 1:13:A:ALA:HB1 | 1:51:A:HIS:H   | 19       | 0.19          |
| (1,60)   | 1:13:A:ALA:HB2 | 1:51:A:HIS:H   | 19       | 0.19          |
| (1,60)   | 1:13:A:ALA:HB3 | 1:51:A:HIS:H   | 19       | 0.19          |
| (1,60)   | 1:13:A:ALA:HB1 | 1:51:A:HIS:H   | 20       | 0.19          |
| (1,60)   | 1:13:A:ALA:HB2 | 1:51:A:HIS:H   | 20       | 0.19          |
| (1,60)   | 1:13:A:ALA:HB3 | 1:51:A:HIS:H   | 20       | 0.19          |
| (1,1309) | 1:87:A:LEU:HB2 | 1:87:A:LEU:H   | 14       | 0.18          |
| (1,1015) | 1:68:A:ALA:HA  | 1:71:A:GLN:HB2 | 14       | 0.18          |
| (1,791)  | 1:52:A:PRO:HD2 | 1:54:A:HIS:H   | 13       | 0.18          |
| (1,194)  | 1:19:A:ARG:H   | 1:20:A:LEU:HG  | 5        | 0.18          |
| (1,30)   | 1:11:A:GLU:HG2 | 1:13:A:ALA:H   | 6        | 0.18          |
| (1,30)   | 1:11:A:GLU:HG3 | 1:13:A:ALA:H   | 6        | 0.18          |
| (1,1015) | 1:68:A:ALA:HA  | 1:71:A:GLN:HB2 | 10       | 0.17          |
| (1,1001) | 1:67:A:LEU:HB3 | 1:67:A:LEU:H   | 12       | 0.17          |
| (1,958)  | 1:64:A:GLU:HB2 | 1:64:A:GLU:H   | 7        | 0.17          |
| (1,948)  | 1:64:A:GLU:HA  | 1:64:A:GLU:H   | 2        | 0.17          |
| (1,948)  | 1:64:A:GLU:HA  | 1:64:A:GLU:H   | 4        | 0.17          |
| (1,948)  | 1:64:A:GLU:HA  | 1:64:A:GLU:H   | 9        | 0.17          |
| (1,914)  | 1:61:A:SER:HB2 | 1:67:A:LEU:HA  | 2        | 0.17          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,914)  | 1:61:A:SER:HB3  | 1:67:A:LEU:HA  | 2        | 0.17          |
| (1,651)  | 1:44:A:SER:HB3  | 1:61:A:SER:HA  | 7        | 0.17          |
| (1,521)  | 1:38:A:PHE:HA   | 1:46:A:CYS:H   | 8        | 0.17          |
| (1,521)  | 1:38:A:PHE:HA   | 1:46:A:CYS:H   | 12       | 0.17          |
| (1,279)  | 1:23:A:HIS:HD2  | 1:25:A:GLY:H   | 1        | 0.17          |
| (1,279)  | 1:23:A:HIS:HD1  | 1:25:A:GLY:H   | 20       | 0.17          |
| (1,160)  | 1:17:A:VAL:HG21 | 1:36:A:ARG:H   | 7        | 0.17          |
| (1,160)  | 1:17:A:VAL:HG22 | 1:36:A:ARG:H   | 7        | 0.17          |
| (1,160)  | 1:17:A:VAL:HG23 | 1:36:A:ARG:H   | 7        | 0.17          |
| (1,113)  | 1:15:A:ARG:HD2  | 1:20:A:LEU:H   | 16       | 0.17          |
| (1,113)  | 1:15:A:ARG:HD3  | 1:20:A:LEU:H   | 16       | 0.17          |
| (1,96)   | 1:15:A:ARG:HA   | 1:19:A:ARG:H   | 5        | 0.17          |
| (1,60)   | 1:13:A:ALA:HB1  | 1:51:A:HIS:H   | 6        | 0.17          |
| (1,60)   | 1:13:A:ALA:HB2  | 1:51:A:HIS:H   | 6        | 0.17          |
| (1,60)   | 1:13:A:ALA:HB3  | 1:51:A:HIS:H   | 6        | 0.17          |
| (1,60)   | 1:13:A:ALA:HB1  | 1:51:A:HIS:H   | 16       | 0.17          |
| (1,60)   | 1:13:A:ALA:HB2  | 1:51:A:HIS:H   | 16       | 0.17          |
| (1,60)   | 1:13:A:ALA:HB3  | 1:51:A:HIS:H   | 16       | 0.17          |
| (1,30)   | 1:11:A:GLU:HG2  | 1:13:A:ALA:H   | 10       | 0.17          |
| (1,30)   | 1:11:A:GLU:HG3  | 1:13:A:ALA:H   | 10       | 0.17          |
| (1,30)   | 1:11:A:GLU:HG2  | 1:13:A:ALA:H   | 14       | 0.17          |
| (1,30)   | 1:11:A:GLU:HG3  | 1:13:A:ALA:H   | 14       | 0.17          |
| (1,30)   | 1:11:A:GLU:HG2  | 1:13:A:ALA:H   | 19       | 0.17          |
| (1,30)   | 1:11:A:GLU:HG3  | 1:13:A:ALA:H   | 19       | 0.17          |
| (1,9)    | 1:10:A:THR:HG21 | 1:53:A:ASP:HA  | 16       | 0.17          |
| (1,9)    | 1:10:A:THR:HG22 | 1:53:A:ASP:HA  | 16       | 0.17          |
| (1,9)    | 1:10:A:THR:HG23 | 1:53:A:ASP:HA  | 16       | 0.17          |
| (1,1309) | 1:87:A:LEU:HB2  | 1:87:A:LEU:H   | 6        | 0.16          |
| (1,1015) | 1:68:A:ALA:HA   | 1:71:A:GLN:HB2 | 8        | 0.16          |
| (1,1015) | 1:68:A:ALA:HA   | 1:71:A:GLN:HB2 | 11       | 0.16          |
| (1,1015) | 1:68:A:ALA:HA   | 1:71:A:GLN:HB2 | 12       | 0.16          |
| (1,1015) | 1:68:A:ALA:HA   | 1:71:A:GLN:HB2 | 13       | 0.16          |
| (1,1015) | 1:68:A:ALA:HA   | 1:71:A:GLN:HB2 | 15       | 0.16          |
| (1,1015) | 1:68:A:ALA:HA   | 1:71:A:GLN:HB2 | 17       | 0.16          |
| (1,1001) | 1:67:A:LEU:HB3  | 1:67:A:LEU:H   | 1        | 0.16          |
| (1,1001) | 1:67:A:LEU:HB3  | 1:67:A:LEU:H   | 3        | 0.16          |
| (1,1001) | 1:67:A:LEU:HB3  | 1:67:A:LEU:H   | 5        | 0.16          |
| (1,1001) | 1:67:A:LEU:HB3  | 1:67:A:LEU:H   | 6        | 0.16          |
| (1,1001) | 1:67:A:LEU:HB3  | 1:67:A:LEU:H   | 7        | 0.16          |
| (1,1001) | 1:67:A:LEU:HB3  | 1:67:A:LEU:H   | 8        | 0.16          |
| (1,1001) | 1:67:A:LEU:HB3  | 1:67:A:LEU:H   | 10       | 0.16          |
| (1,1001) | 1:67:A:LEU:HB3  | 1:67:A:LEU:H   | 11       | 0.16          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1001) | 1:67:A:LEU:HB3 | 1:67:A:LEU:H   | 18       | 0.16          |
| (1,958)  | 1:64:A:GLU:HB2 | 1:64:A:GLU:H   | 1        | 0.16          |
| (1,958)  | 1:64:A:GLU:HB2 | 1:64:A:GLU:H   | 3        | 0.16          |
| (1,958)  | 1:64:A:GLU:HB2 | 1:64:A:GLU:H   | 4        | 0.16          |
| (1,958)  | 1:64:A:GLU:HB2 | 1:64:A:GLU:H   | 5        | 0.16          |
| (1,958)  | 1:64:A:GLU:HB2 | 1:64:A:GLU:H   | 6        | 0.16          |
| (1,958)  | 1:64:A:GLU:HB2 | 1:64:A:GLU:H   | 8        | 0.16          |
| (1,958)  | 1:64:A:GLU:HB2 | 1:64:A:GLU:H   | 10       | 0.16          |
| (1,958)  | 1:64:A:GLU:HB2 | 1:64:A:GLU:H   | 11       | 0.16          |
| (1,958)  | 1:64:A:GLU:HB2 | 1:64:A:GLU:H   | 12       | 0.16          |
| (1,958)  | 1:64:A:GLU:HB2 | 1:64:A:GLU:H   | 13       | 0.16          |
| (1,958)  | 1:64:A:GLU:HB2 | 1:64:A:GLU:H   | 15       | 0.16          |
| (1,958)  | 1:64:A:GLU:HB2 | 1:64:A:GLU:H   | 16       | 0.16          |
| (1,958)  | 1:64:A:GLU:HB2 | 1:64:A:GLU:H   | 17       | 0.16          |
| (1,958)  | 1:64:A:GLU:HB2 | 1:64:A:GLU:H   | 18       | 0.16          |
| (1,958)  | 1:64:A:GLU:HB2 | 1:64:A:GLU:H   | 19       | 0.16          |
| (1,958)  | 1:64:A:GLU:HB2 | 1:64:A:GLU:H   | 20       | 0.16          |
| (1,948)  | 1:64:A:GLU:HA  | 1:64:A:GLU:H   | 1        | 0.16          |
| (1,948)  | 1:64:A:GLU:HA  | 1:64:A:GLU:H   | 3        | 0.16          |
| (1,948)  | 1:64:A:GLU:HA  | 1:64:A:GLU:H   | 5        | 0.16          |
| (1,948)  | 1:64:A:GLU:HA  | 1:64:A:GLU:H   | 6        | 0.16          |
| (1,948)  | 1:64:A:GLU:HA  | 1:64:A:GLU:H   | 8        | 0.16          |
| (1,948)  | 1:64:A:GLU:HA  | 1:64:A:GLU:H   | 10       | 0.16          |
| (1,948)  | 1:64:A:GLU:HA  | 1:64:A:GLU:H   | 11       | 0.16          |
| (1,948)  | 1:64:A:GLU:HA  | 1:64:A:GLU:H   | 13       | 0.16          |
| (1,948)  | 1:64:A:GLU:HA  | 1:64:A:GLU:H   | 15       | 0.16          |
| (1,948)  | 1:64:A:GLU:HA  | 1:64:A:GLU:H   | 16       | 0.16          |
| (1,948)  | 1:64:A:GLU:HA  | 1:64:A:GLU:H   | 17       | 0.16          |
| (1,948)  | 1:64:A:GLU:HA  | 1:64:A:GLU:H   | 18       | 0.16          |
| (1,948)  | 1:64:A:GLU:HA  | 1:64:A:GLU:H   | 20       | 0.16          |
| (1,914)  | 1:61:A:SER:HB2 | 1:67:A:LEU:HA  | 1        | 0.16          |
| (1,914)  | 1:61:A:SER:HB3 | 1:67:A:LEU:HA  | 1        | 0.16          |
| (1,914)  | 1:61:A:SER:HB2 | 1:67:A:LEU:HA  | 7        | 0.16          |
| (1,914)  | 1:61:A:SER:HB3 | 1:67:A:LEU:HA  | 7        | 0.16          |
| (1,914)  | 1:61:A:SER:HB2 | 1:67:A:LEU:HA  | 9        | 0.16          |
| (1,914)  | 1:61:A:SER:HB3 | 1:67:A:LEU:HA  | 9        | 0.16          |
| (1,704)  | 1:48:A:LEU:HB2 | 1:48:A:LEU:H   | 20       | 0.16          |
| (1,704)  | 1:48:A:LEU:HB3 | 1:48:A:LEU:H   | 20       | 0.16          |
| (1,673)  | 1:45:A:ASN:H   | 1:70:A:MET:HB3 | 12       | 0.16          |
| (1,521)  | 1:38:A:PHE:HA  | 1:46:A:CYS:H   | 6        | 0.16          |
| (1,521)  | 1:38:A:PHE:HA  | 1:46:A:CYS:H   | 11       | 0.16          |
| (1,511)  | 1:37:A:GLY:HA2 | 1:38:A:PHE:H   | 1        | 0.16          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,511) | 1:37:A:GLY:HA2  | 1:38:A:PHE:H   | 4        | 0.16          |
| (1,511) | 1:37:A:GLY:HA2  | 1:38:A:PHE:H   | 5        | 0.16          |
| (1,511) | 1:37:A:GLY:HA2  | 1:38:A:PHE:H   | 6        | 0.16          |
| (1,511) | 1:37:A:GLY:HA2  | 1:38:A:PHE:H   | 8        | 0.16          |
| (1,511) | 1:37:A:GLY:HA2  | 1:38:A:PHE:H   | 9        | 0.16          |
| (1,511) | 1:37:A:GLY:HA2  | 1:38:A:PHE:H   | 11       | 0.16          |
| (1,511) | 1:37:A:GLY:HA2  | 1:38:A:PHE:H   | 12       | 0.16          |
| (1,511) | 1:37:A:GLY:HA2  | 1:38:A:PHE:H   | 14       | 0.16          |
| (1,511) | 1:37:A:GLY:HA2  | 1:38:A:PHE:H   | 15       | 0.16          |
| (1,511) | 1:37:A:GLY:HA2  | 1:38:A:PHE:H   | 19       | 0.16          |
| (1,493) | 1:36:A:ARG:HA   | 1:49:A:LEU:HA  | 20       | 0.16          |
| (1,279) | 1:23:A:HIS:HD2  | 1:25:A:GLY:H   | 16       | 0.16          |
| (1,261) | 1:22:A:LYS:HE2  | 1:22:A:LYS:HG2 | 17       | 0.16          |
| (1,261) | 1:22:A:LYS:HE2  | 1:22:A:LYS:HG3 | 17       | 0.16          |
| (1,261) | 1:22:A:LYS:HE3  | 1:22:A:LYS:HG2 | 17       | 0.16          |
| (1,261) | 1:22:A:LYS:HE3  | 1:22:A:LYS:HG3 | 17       | 0.16          |
| (1,194) | 1:19:A:ARG:H    | 1:20:A:LEU:HG  | 6        | 0.16          |
| (1,160) | 1:17:A:VAL:HG21 | 1:36:A:ARG:H   | 10       | 0.16          |
| (1,160) | 1:17:A:VAL:HG22 | 1:36:A:ARG:H   | 10       | 0.16          |
| (1,160) | 1:17:A:VAL:HG23 | 1:36:A:ARG:H   | 10       | 0.16          |
| (1,160) | 1:17:A:VAL:HG21 | 1:36:A:ARG:H   | 17       | 0.16          |
| (1,160) | 1:17:A:VAL:HG22 | 1:36:A:ARG:H   | 17       | 0.16          |
| (1,160) | 1:17:A:VAL:HG23 | 1:36:A:ARG:H   | 17       | 0.16          |
| (1,120) | 1:16:A:TYR:HA   | 1:16:A:TYR:HD1 | 2        | 0.16          |
| (1,120) | 1:16:A:TYR:HA   | 1:16:A:TYR:HD2 | 2        | 0.16          |
| (1,120) | 1:16:A:TYR:HA   | 1:16:A:TYR:HD1 | 3        | 0.16          |
| (1,120) | 1:16:A:TYR:HA   | 1:16:A:TYR:HD2 | 3        | 0.16          |
| (1,120) | 1:16:A:TYR:HA   | 1:16:A:TYR:HD1 | 4        | 0.16          |
| (1,120) | 1:16:A:TYR:HA   | 1:16:A:TYR:HD2 | 4        | 0.16          |
| (1,120) | 1:16:A:TYR:HA   | 1:16:A:TYR:HD1 | 10       | 0.16          |
| (1,120) | 1:16:A:TYR:HA   | 1:16:A:TYR:HD2 | 10       | 0.16          |
| (1,120) | 1:16:A:TYR:HA   | 1:16:A:TYR:HD1 | 11       | 0.16          |
| (1,120) | 1:16:A:TYR:HA   | 1:16:A:TYR:HD2 | 11       | 0.16          |
| (1,120) | 1:16:A:TYR:HA   | 1:16:A:TYR:HD1 | 12       | 0.16          |
| (1,120) | 1:16:A:TYR:HA   | 1:16:A:TYR:HD2 | 12       | 0.16          |
| (1,120) | 1:16:A:TYR:HA   | 1:16:A:TYR:HD1 | 13       | 0.16          |
| (1,120) | 1:16:A:TYR:HA   | 1:16:A:TYR:HD2 | 13       | 0.16          |
| (1,120) | 1:16:A:TYR:HA   | 1:16:A:TYR:HD1 | 14       | 0.16          |
| (1,120) | 1:16:A:TYR:HA   | 1:16:A:TYR:HD2 | 14       | 0.16          |
| (1,30)  | 1:11:A:GLU:HG2  | 1:13:A:ALA:H   | 1        | 0.16          |
| (1,30)  | 1:11:A:GLU:HG3  | 1:13:A:ALA:H   | 1        | 0.16          |
| (1,30)  | 1:11:A:GLU:HG2  | 1:13:A:ALA:H   | 2        | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,30)   | 1:11:A:GLU:HG3  | 1:13:A:ALA:H    | 2        | 0.16          |
| (1,30)   | 1:11:A:GLU:HG2  | 1:13:A:ALA:H    | 3        | 0.16          |
| (1,30)   | 1:11:A:GLU:HG3  | 1:13:A:ALA:H    | 3        | 0.16          |
| (1,30)   | 1:11:A:GLU:HG2  | 1:13:A:ALA:H    | 4        | 0.16          |
| (1,30)   | 1:11:A:GLU:HG3  | 1:13:A:ALA:H    | 4        | 0.16          |
| (1,30)   | 1:11:A:GLU:HG2  | 1:13:A:ALA:H    | 5        | 0.16          |
| (1,30)   | 1:11:A:GLU:HG3  | 1:13:A:ALA:H    | 5        | 0.16          |
| (1,30)   | 1:11:A:GLU:HG2  | 1:13:A:ALA:H    | 8        | 0.16          |
| (1,30)   | 1:11:A:GLU:HG3  | 1:13:A:ALA:H    | 8        | 0.16          |
| (1,30)   | 1:11:A:GLU:HG2  | 1:13:A:ALA:H    | 11       | 0.16          |
| (1,30)   | 1:11:A:GLU:HG3  | 1:13:A:ALA:H    | 11       | 0.16          |
| (1,30)   | 1:11:A:GLU:HG2  | 1:13:A:ALA:H    | 12       | 0.16          |
| (1,30)   | 1:11:A:GLU:HG3  | 1:13:A:ALA:H    | 12       | 0.16          |
| (1,30)   | 1:11:A:GLU:HG2  | 1:13:A:ALA:H    | 15       | 0.16          |
| (1,30)   | 1:11:A:GLU:HG3  | 1:13:A:ALA:H    | 15       | 0.16          |
| (1,30)   | 1:11:A:GLU:HG2  | 1:13:A:ALA:H    | 16       | 0.16          |
| (1,30)   | 1:11:A:GLU:HG3  | 1:13:A:ALA:H    | 16       | 0.16          |
| (1,30)   | 1:11:A:GLU:HG2  | 1:13:A:ALA:H    | 18       | 0.16          |
| (1,30)   | 1:11:A:GLU:HG3  | 1:13:A:ALA:H    | 18       | 0.16          |
| (1,30)   | 1:11:A:GLU:HG2  | 1:13:A:ALA:H    | 20       | 0.16          |
| (1,30)   | 1:11:A:GLU:HG3  | 1:13:A:ALA:H    | 20       | 0.16          |
| (1,9)    | 1:10:A:THR:HG21 | 1:53:A:ASP:HA   | 13       | 0.16          |
| (1,9)    | 1:10:A:THR:HG22 | 1:53:A:ASP:HA   | 13       | 0.16          |
| (1,9)    | 1:10:A:THR:HG23 | 1:53:A:ASP:HA   | 13       | 0.16          |
| (1,9)    | 1:10:A:THR:HG21 | 1:53:A:ASP:HA   | 14       | 0.16          |
| (1,9)    | 1:10:A:THR:HG22 | 1:53:A:ASP:HA   | 14       | 0.16          |
| (1,9)    | 1:10:A:THR:HG23 | 1:53:A:ASP:HA   | 14       | 0.16          |
| (1,1342) | 1:90:A:ALA:HB1  | 1:90:A:ALA:H    | 6        | 0.15          |
| (1,1342) | 1:90:A:ALA:HB2  | 1:90:A:ALA:H    | 6        | 0.15          |
| (1,1342) | 1:90:A:ALA:HB3  | 1:90:A:ALA:H    | 6        | 0.15          |
| (1,1174) | 1:75:A:ALA:HB1  | 1:89:A:ILE:HD11 | 13       | 0.15          |
| (1,1174) | 1:75:A:ALA:HB1  | 1:89:A:ILE:HD12 | 13       | 0.15          |
| (1,1174) | 1:75:A:ALA:HB1  | 1:89:A:ILE:HD13 | 13       | 0.15          |
| (1,1174) | 1:75:A:ALA:HB2  | 1:89:A:ILE:HD11 | 13       | 0.15          |
| (1,1174) | 1:75:A:ALA:HB2  | 1:89:A:ILE:HD12 | 13       | 0.15          |
| (1,1174) | 1:75:A:ALA:HB2  | 1:89:A:ILE:HD13 | 13       | 0.15          |
| (1,1174) | 1:75:A:ALA:HB3  | 1:89:A:ILE:HD11 | 13       | 0.15          |
| (1,1174) | 1:75:A:ALA:HB3  | 1:89:A:ILE:HD12 | 13       | 0.15          |
| (1,1174) | 1:75:A:ALA:HB3  | 1:89:A:ILE:HD13 | 13       | 0.15          |
| (1,1145) | 1:74:A:VAL:HB   | 1:76:A:ASP:H    | 13       | 0.15          |
| (1,1015) | 1:68:A:ALA:HA   | 1:71:A:GLN:HB2  | 1        | 0.15          |
| (1,1015) | 1:68:A:ALA:HA   | 1:71:A:GLN:HB2  | 3        | 0.15          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1015) | 1:68:A:ALA:HA  | 1:71:A:GLN:HB2  | 5        | 0.15          |
| (1,1015) | 1:68:A:ALA:HA  | 1:71:A:GLN:HB2  | 6        | 0.15          |
| (1,1015) | 1:68:A:ALA:HA  | 1:71:A:GLN:HB2  | 16       | 0.15          |
| (1,1015) | 1:68:A:ALA:HA  | 1:71:A:GLN:HB2  | 19       | 0.15          |
| (1,1015) | 1:68:A:ALA:HA  | 1:71:A:GLN:HB2  | 20       | 0.15          |
| (1,1001) | 1:67:A:LEU:HB3 | 1:67:A:LEU:H    | 4        | 0.15          |
| (1,1001) | 1:67:A:LEU:HB3 | 1:67:A:LEU:H    | 13       | 0.15          |
| (1,1001) | 1:67:A:LEU:HB3 | 1:67:A:LEU:H    | 15       | 0.15          |
| (1,1001) | 1:67:A:LEU:HB3 | 1:67:A:LEU:H    | 16       | 0.15          |
| (1,1001) | 1:67:A:LEU:HB3 | 1:67:A:LEU:H    | 17       | 0.15          |
| (1,1001) | 1:67:A:LEU:HB3 | 1:67:A:LEU:H    | 20       | 0.15          |
| (1,958)  | 1:64:A:GLU:HB2 | 1:64:A:GLU:H    | 2        | 0.15          |
| (1,958)  | 1:64:A:GLU:HB2 | 1:64:A:GLU:H    | 9        | 0.15          |
| (1,958)  | 1:64:A:GLU:HB2 | 1:64:A:GLU:H    | 14       | 0.15          |
| (1,948)  | 1:64:A:GLU:HA  | 1:64:A:GLU:H    | 7        | 0.15          |
| (1,948)  | 1:64:A:GLU:HA  | 1:64:A:GLU:H    | 12       | 0.15          |
| (1,948)  | 1:64:A:GLU:HA  | 1:64:A:GLU:H    | 14       | 0.15          |
| (1,948)  | 1:64:A:GLU:HA  | 1:64:A:GLU:H    | 19       | 0.15          |
| (1,942)  | 1:63:A:ASP:H   | 1:67:A:LEU:HB3  | 12       | 0.15          |
| (1,922)  | 1:62:A:PRO:HB3 | 1:63:A:ASP:H    | 9        | 0.15          |
| (1,922)  | 1:62:A:PRO:HB3 | 1:63:A:ASP:H    | 20       | 0.15          |
| (1,914)  | 1:61:A:SER:HB2 | 1:67:A:LEU:HA   | 17       | 0.15          |
| (1,914)  | 1:61:A:SER:HB3 | 1:67:A:LEU:HA   | 17       | 0.15          |
| (1,914)  | 1:61:A:SER:HB2 | 1:67:A:LEU:HA   | 18       | 0.15          |
| (1,914)  | 1:61:A:SER:HB3 | 1:67:A:LEU:HA   | 18       | 0.15          |
| (1,914)  | 1:61:A:SER:HB2 | 1:67:A:LEU:HA   | 20       | 0.15          |
| (1,914)  | 1:61:A:SER:HB3 | 1:67:A:LEU:HA   | 20       | 0.15          |
| (1,808)  | 1:54:A:HIS:HD1 | 1:56:A:LEU:HD12 | 5        | 0.15          |
| (1,726)  | 1:49:A:LEU:H   | 1:57:A:MET:HG2  | 2        | 0.15          |
| (1,726)  | 1:49:A:LEU:H   | 1:57:A:MET:HG2  | 7        | 0.15          |
| (1,726)  | 1:49:A:LEU:H   | 1:57:A:MET:HG2  | 16       | 0.15          |
| (1,704)  | 1:48:A:LEU:HB2 | 1:48:A:LEU:H    | 5        | 0.15          |
| (1,704)  | 1:48:A:LEU:HB3 | 1:48:A:LEU:H    | 5        | 0.15          |
| (1,673)  | 1:45:A:ASN:H   | 1:70:A:MET:HB3  | 15       | 0.15          |
| (1,673)  | 1:45:A:ASN:H   | 1:70:A:MET:HB3  | 17       | 0.15          |
| (1,589)  | 1:3:A:ARG:HB2  | 1:3:A:ARG:H     | 8        | 0.15          |
| (1,589)  | 1:3:A:ARG:HB3  | 1:3:A:ARG:H     | 8        | 0.15          |
| (1,589)  | 1:3:A:ARG:HB2  | 1:3:A:ARG:H     | 9        | 0.15          |
| (1,589)  | 1:3:A:ARG:HB3  | 1:3:A:ARG:H     | 9        | 0.15          |
| (1,521)  | 1:38:A:PHE:HA  | 1:46:A:CYS:H    | 3        | 0.15          |
| (1,521)  | 1:38:A:PHE:HA  | 1:46:A:CYS:H    | 15       | 0.15          |
| (1,521)  | 1:38:A:PHE:HA  | 1:46:A:CYS:H    | 16       | 0.15          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,194)  | 1:19:A:ARG:H    | 1:20:A:LEU:HG  | 4        | 0.15          |
| (1,194)  | 1:19:A:ARG:H    | 1:20:A:LEU:HG  | 11       | 0.15          |
| (1,194)  | 1:19:A:ARG:H    | 1:20:A:LEU:HG  | 14       | 0.15          |
| (1,160)  | 1:17:A:VAL:HG21 | 1:36:A:ARG:H   | 2        | 0.15          |
| (1,160)  | 1:17:A:VAL:HG22 | 1:36:A:ARG:H   | 2        | 0.15          |
| (1,160)  | 1:17:A:VAL:HG23 | 1:36:A:ARG:H   | 2        | 0.15          |
| (1,160)  | 1:17:A:VAL:HG21 | 1:36:A:ARG:H   | 16       | 0.15          |
| (1,160)  | 1:17:A:VAL:HG22 | 1:36:A:ARG:H   | 16       | 0.15          |
| (1,160)  | 1:17:A:VAL:HG23 | 1:36:A:ARG:H   | 16       | 0.15          |
| (1,120)  | 1:16:A:TYR:HA   | 1:16:A:TYR:HD1 | 1        | 0.15          |
| (1,120)  | 1:16:A:TYR:HA   | 1:16:A:TYR:HD2 | 1        | 0.15          |
| (1,120)  | 1:16:A:TYR:HA   | 1:16:A:TYR:HD1 | 7        | 0.15          |
| (1,120)  | 1:16:A:TYR:HA   | 1:16:A:TYR:HD2 | 7        | 0.15          |
| (1,120)  | 1:16:A:TYR:HA   | 1:16:A:TYR:HD1 | 8        | 0.15          |
| (1,120)  | 1:16:A:TYR:HA   | 1:16:A:TYR:HD2 | 8        | 0.15          |
| (1,120)  | 1:16:A:TYR:HA   | 1:16:A:TYR:HD1 | 9        | 0.15          |
| (1,120)  | 1:16:A:TYR:HA   | 1:16:A:TYR:HD2 | 9        | 0.15          |
| (1,120)  | 1:16:A:TYR:HA   | 1:16:A:TYR:HD1 | 15       | 0.15          |
| (1,120)  | 1:16:A:TYR:HA   | 1:16:A:TYR:HD2 | 15       | 0.15          |
| (1,120)  | 1:16:A:TYR:HA   | 1:16:A:TYR:HD1 | 19       | 0.15          |
| (1,120)  | 1:16:A:TYR:HA   | 1:16:A:TYR:HD2 | 19       | 0.15          |
| (1,96)   | 1:15:A:ARG:HA   | 1:19:A:ARG:H   | 6        | 0.15          |
| (1,30)   | 1:11:A:GLU:HG2  | 1:13:A:ALA:H   | 7        | 0.15          |
| (1,30)   | 1:11:A:GLU:HG3  | 1:13:A:ALA:H   | 7        | 0.15          |
| (1,30)   | 1:11:A:GLU:HG2  | 1:13:A:ALA:H   | 9        | 0.15          |
| (1,30)   | 1:11:A:GLU:HG3  | 1:13:A:ALA:H   | 9        | 0.15          |
| (1,30)   | 1:11:A:GLU:HG2  | 1:13:A:ALA:H   | 13       | 0.15          |
| (1,30)   | 1:11:A:GLU:HG3  | 1:13:A:ALA:H   | 13       | 0.15          |
| (1,30)   | 1:11:A:GLU:HG2  | 1:13:A:ALA:H   | 17       | 0.15          |
| (1,30)   | 1:11:A:GLU:HG3  | 1:13:A:ALA:H   | 17       | 0.15          |
| (1,1328) | 1:89:A:ILE:HG21 | 1:91:A:TRP:H   | 11       | 0.14          |
| (1,1328) | 1:89:A:ILE:HG22 | 1:91:A:TRP:H   | 11       | 0.14          |
| (1,1328) | 1:89:A:ILE:HG23 | 1:91:A:TRP:H   | 11       | 0.14          |
| (1,1328) | 1:89:A:ILE:HG21 | 1:91:A:TRP:H   | 12       | 0.14          |
| (1,1328) | 1:89:A:ILE:HG22 | 1:91:A:TRP:H   | 12       | 0.14          |
| (1,1328) | 1:89:A:ILE:HG23 | 1:91:A:TRP:H   | 12       | 0.14          |
| (1,1328) | 1:89:A:ILE:HG21 | 1:91:A:TRP:H   | 15       | 0.14          |
| (1,1328) | 1:89:A:ILE:HG22 | 1:91:A:TRP:H   | 15       | 0.14          |
| (1,1328) | 1:89:A:ILE:HG23 | 1:91:A:TRP:H   | 15       | 0.14          |
| (1,1328) | 1:89:A:ILE:HG21 | 1:91:A:TRP:H   | 19       | 0.14          |
| (1,1328) | 1:89:A:ILE:HG22 | 1:91:A:TRP:H   | 19       | 0.14          |
| (1,1328) | 1:89:A:ILE:HG23 | 1:91:A:TRP:H   | 19       | 0.14          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1328) | 1:89:A:ILE:HG21 | 1:91:A:TRP:H   | 20       | 0.14          |
| (1,1328) | 1:89:A:ILE:HG22 | 1:91:A:TRP:H   | 20       | 0.14          |
| (1,1328) | 1:89:A:ILE:HG23 | 1:91:A:TRP:H   | 20       | 0.14          |
| (1,1309) | 1:87:A:LEU:HB2  | 1:87:A:LEU:H   | 4        | 0.14          |
| (1,1309) | 1:87:A:LEU:HB2  | 1:87:A:LEU:H   | 19       | 0.14          |
| (1,1139) | 1:74:A:VAL:HA   | 1:77:A:HIS:HB2 | 19       | 0.14          |
| (1,1139) | 1:74:A:VAL:HA   | 1:77:A:HIS:HB2 | 20       | 0.14          |
| (1,1138) | 1:74:A:VAL:HA   | 1:77:A:HIS:HB3 | 19       | 0.14          |
| (1,1138) | 1:74:A:VAL:HA   | 1:77:A:HIS:HB3 | 20       | 0.14          |
| (1,1015) | 1:68:A:ALA:HA   | 1:71:A:GLN:HB2 | 4        | 0.14          |
| (1,1015) | 1:68:A:ALA:HA   | 1:71:A:GLN:HB2 | 7        | 0.14          |
| (1,1015) | 1:68:A:ALA:HA   | 1:71:A:GLN:HB2 | 18       | 0.14          |
| (1,954)  | 1:64:A:GLU:HA   | 1:67:A:LEU:HG  | 7        | 0.14          |
| (1,942)  | 1:63:A:ASP:H    | 1:67:A:LEU:HB3 | 2        | 0.14          |
| (1,942)  | 1:63:A:ASP:H    | 1:67:A:LEU:HB3 | 8        | 0.14          |
| (1,942)  | 1:63:A:ASP:H    | 1:67:A:LEU:HB3 | 19       | 0.14          |
| (1,942)  | 1:63:A:ASP:H    | 1:67:A:LEU:HB3 | 20       | 0.14          |
| (1,922)  | 1:62:A:PRO:HB3  | 1:63:A:ASP:H   | 1        | 0.14          |
| (1,922)  | 1:62:A:PRO:HB3  | 1:63:A:ASP:H   | 2        | 0.14          |
| (1,922)  | 1:62:A:PRO:HB3  | 1:63:A:ASP:H   | 5        | 0.14          |
| (1,922)  | 1:62:A:PRO:HB3  | 1:63:A:ASP:H   | 11       | 0.14          |
| (1,922)  | 1:62:A:PRO:HB3  | 1:63:A:ASP:H   | 12       | 0.14          |
| (1,922)  | 1:62:A:PRO:HB3  | 1:63:A:ASP:H   | 13       | 0.14          |
| (1,922)  | 1:62:A:PRO:HB3  | 1:63:A:ASP:H   | 17       | 0.14          |
| (1,922)  | 1:62:A:PRO:HB3  | 1:63:A:ASP:H   | 18       | 0.14          |
| (1,914)  | 1:61:A:SER:HB2  | 1:67:A:LEU:HA  | 4        | 0.14          |
| (1,914)  | 1:61:A:SER:HB3  | 1:67:A:LEU:HA  | 4        | 0.14          |
| (1,878)  | 1:5:A:THR:HA    | 1:5:A:THR:HG21 | 1        | 0.14          |
| (1,878)  | 1:5:A:THR:HA    | 1:5:A:THR:HG22 | 1        | 0.14          |
| (1,878)  | 1:5:A:THR:HA    | 1:5:A:THR:HG23 | 1        | 0.14          |
| (1,878)  | 1:5:A:THR:HA    | 1:5:A:THR:HG21 | 3        | 0.14          |
| (1,878)  | 1:5:A:THR:HA    | 1:5:A:THR:HG22 | 3        | 0.14          |
| (1,878)  | 1:5:A:THR:HA    | 1:5:A:THR:HG23 | 3        | 0.14          |
| (1,878)  | 1:5:A:THR:HA    | 1:5:A:THR:HG21 | 8        | 0.14          |
| (1,878)  | 1:5:A:THR:HA    | 1:5:A:THR:HG22 | 8        | 0.14          |
| (1,878)  | 1:5:A:THR:HA    | 1:5:A:THR:HG23 | 8        | 0.14          |
| (1,878)  | 1:5:A:THR:HA    | 1:5:A:THR:HG21 | 12       | 0.14          |
| (1,878)  | 1:5:A:THR:HA    | 1:5:A:THR:HG22 | 12       | 0.14          |
| (1,878)  | 1:5:A:THR:HA    | 1:5:A:THR:HG23 | 12       | 0.14          |
| (1,878)  | 1:5:A:THR:HA    | 1:5:A:THR:HG21 | 13       | 0.14          |
| (1,878)  | 1:5:A:THR:HA    | 1:5:A:THR:HG22 | 13       | 0.14          |
| (1,878)  | 1:5:A:THR:HA    | 1:5:A:THR:HG23 | 13       | 0.14          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG21  | 15       | 0.14          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG22  | 15       | 0.14          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG23  | 15       | 0.14          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG21  | 18       | 0.14          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG22  | 18       | 0.14          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG23  | 18       | 0.14          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG21  | 20       | 0.14          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG22  | 20       | 0.14          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG23  | 20       | 0.14          |
| (1,808) | 1:54:A:HIS:HD1 | 1:56:A:LEU:HD11 | 17       | 0.14          |
| (1,744) | 1:4:A:SER:HB2  | 1:93:A:PRO:HB2  | 1        | 0.14          |
| (1,744) | 1:4:A:SER:HB3  | 1:93:A:PRO:HB2  | 1        | 0.14          |
| (1,744) | 1:4:A:SER:HB2  | 1:93:A:PRO:HB2  | 2        | 0.14          |
| (1,744) | 1:4:A:SER:HB3  | 1:93:A:PRO:HB2  | 2        | 0.14          |
| (1,744) | 1:4:A:SER:HB2  | 1:93:A:PRO:HB2  | 3        | 0.14          |
| (1,744) | 1:4:A:SER:HB3  | 1:93:A:PRO:HB2  | 3        | 0.14          |
| (1,744) | 1:4:A:SER:HB2  | 1:93:A:PRO:HB2  | 7        | 0.14          |
| (1,744) | 1:4:A:SER:HB3  | 1:93:A:PRO:HB2  | 7        | 0.14          |
| (1,744) | 1:4:A:SER:HB2  | 1:93:A:PRO:HB2  | 9        | 0.14          |
| (1,744) | 1:4:A:SER:HB3  | 1:93:A:PRO:HB2  | 9        | 0.14          |
| (1,744) | 1:4:A:SER:HB2  | 1:93:A:PRO:HB2  | 13       | 0.14          |
| (1,744) | 1:4:A:SER:HB3  | 1:93:A:PRO:HB2  | 13       | 0.14          |
| (1,726) | 1:49:A:LEU:H   | 1:57:A:MET:HG2  | 4        | 0.14          |
| (1,726) | 1:49:A:LEU:H   | 1:57:A:MET:HG2  | 6        | 0.14          |
| (1,726) | 1:49:A:LEU:H   | 1:57:A:MET:HG2  | 12       | 0.14          |
| (1,726) | 1:49:A:LEU:H   | 1:57:A:MET:HG2  | 13       | 0.14          |
| (1,726) | 1:49:A:LEU:H   | 1:57:A:MET:HG2  | 14       | 0.14          |
| (1,726) | 1:49:A:LEU:H   | 1:57:A:MET:HG2  | 17       | 0.14          |
| (1,726) | 1:49:A:LEU:H   | 1:57:A:MET:HG2  | 18       | 0.14          |
| (1,704) | 1:48:A:LEU:HB2 | 1:48:A:LEU:H    | 1        | 0.14          |
| (1,704) | 1:48:A:LEU:HB3 | 1:48:A:LEU:H    | 1        | 0.14          |
| (1,704) | 1:48:A:LEU:HB2 | 1:48:A:LEU:H    | 4        | 0.14          |
| (1,704) | 1:48:A:LEU:HB3 | 1:48:A:LEU:H    | 4        | 0.14          |
| (1,704) | 1:48:A:LEU:HB2 | 1:48:A:LEU:H    | 19       | 0.14          |
| (1,704) | 1:48:A:LEU:HB3 | 1:48:A:LEU:H    | 19       | 0.14          |
| (1,673) | 1:45:A:ASN:H   | 1:70:A:MET:HB3  | 3        | 0.14          |
| (1,673) | 1:45:A:ASN:H   | 1:70:A:MET:HB3  | 8        | 0.14          |
| (1,673) | 1:45:A:ASN:H   | 1:70:A:MET:HB3  | 11       | 0.14          |
| (1,673) | 1:45:A:ASN:H   | 1:70:A:MET:HB3  | 18       | 0.14          |
| (1,589) | 1:3:A:ARG:HB2  | 1:3:A:ARG:H     | 1        | 0.14          |
| (1,589) | 1:3:A:ARG:HB3  | 1:3:A:ARG:H     | 1        | 0.14          |
| (1,589) | 1:3:A:ARG:HB2  | 1:3:A:ARG:H     | 2        | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,589) | 1:3:A:ARG:HB3   | 1:3:A:ARG:H     | 2        | 0.14          |
| (1,589) | 1:3:A:ARG:HB2   | 1:3:A:ARG:H     | 3        | 0.14          |
| (1,589) | 1:3:A:ARG:HB3   | 1:3:A:ARG:H     | 3        | 0.14          |
| (1,589) | 1:3:A:ARG:HB2   | 1:3:A:ARG:H     | 6        | 0.14          |
| (1,589) | 1:3:A:ARG:HB3   | 1:3:A:ARG:H     | 6        | 0.14          |
| (1,589) | 1:3:A:ARG:HB2   | 1:3:A:ARG:H     | 7        | 0.14          |
| (1,589) | 1:3:A:ARG:HB3   | 1:3:A:ARG:H     | 7        | 0.14          |
| (1,589) | 1:3:A:ARG:HB2   | 1:3:A:ARG:H     | 15       | 0.14          |
| (1,589) | 1:3:A:ARG:HB3   | 1:3:A:ARG:H     | 15       | 0.14          |
| (1,589) | 1:3:A:ARG:HB2   | 1:3:A:ARG:H     | 18       | 0.14          |
| (1,589) | 1:3:A:ARG:HB3   | 1:3:A:ARG:H     | 18       | 0.14          |
| (1,589) | 1:3:A:ARG:HB2   | 1:3:A:ARG:H     | 20       | 0.14          |
| (1,589) | 1:3:A:ARG:HB3   | 1:3:A:ARG:H     | 20       | 0.14          |
| (1,521) | 1:38:A:PHE:HA   | 1:46:A:CYS:H    | 13       | 0.14          |
| (1,372) | 1:29:A:GLU:H    | 1:41:A:PHE:HA   | 1        | 0.14          |
| (1,292) | 1:24:A:TRP:HB2  | 1:39:A:ILE:HG21 | 20       | 0.14          |
| (1,292) | 1:24:A:TRP:HB2  | 1:39:A:ILE:HG22 | 20       | 0.14          |
| (1,292) | 1:24:A:TRP:HB2  | 1:39:A:ILE:HG23 | 20       | 0.14          |
| (1,292) | 1:24:A:TRP:HB3  | 1:39:A:ILE:HG21 | 20       | 0.14          |
| (1,292) | 1:24:A:TRP:HB3  | 1:39:A:ILE:HG22 | 20       | 0.14          |
| (1,292) | 1:24:A:TRP:HB3  | 1:39:A:ILE:HG23 | 20       | 0.14          |
| (1,194) | 1:19:A:ARG:H    | 1:20:A:LEU:HG   | 8        | 0.14          |
| (1,194) | 1:19:A:ARG:H    | 1:20:A:LEU:HG   | 12       | 0.14          |
| (1,194) | 1:19:A:ARG:H    | 1:20:A:LEU:HG   | 15       | 0.14          |
| (1,194) | 1:19:A:ARG:H    | 1:20:A:LEU:HG   | 19       | 0.14          |
| (1,176) | 1:18:A:ASN:H    | 1:19:A:ARG:H    | 5        | 0.14          |
| (1,176) | 1:18:A:ASN:H    | 1:19:A:ARG:H    | 18       | 0.14          |
| (1,160) | 1:17:A:VAL:HG21 | 1:36:A:ARG:H    | 13       | 0.14          |
| (1,160) | 1:17:A:VAL:HG22 | 1:36:A:ARG:H    | 13       | 0.14          |
| (1,160) | 1:17:A:VAL:HG23 | 1:36:A:ARG:H    | 13       | 0.14          |
| (1,151) | 1:17:A:VAL:HG11 | 1:18:A:ASN:H    | 1        | 0.14          |
| (1,151) | 1:17:A:VAL:HG12 | 1:18:A:ASN:H    | 1        | 0.14          |
| (1,151) | 1:17:A:VAL:HG13 | 1:18:A:ASN:H    | 1        | 0.14          |
| (1,151) | 1:17:A:VAL:HG11 | 1:18:A:ASN:H    | 9        | 0.14          |
| (1,151) | 1:17:A:VAL:HG12 | 1:18:A:ASN:H    | 9        | 0.14          |
| (1,151) | 1:17:A:VAL:HG13 | 1:18:A:ASN:H    | 9        | 0.14          |
| (1,151) | 1:17:A:VAL:HG11 | 1:18:A:ASN:H    | 19       | 0.14          |
| (1,151) | 1:17:A:VAL:HG12 | 1:18:A:ASN:H    | 19       | 0.14          |
| (1,151) | 1:17:A:VAL:HG13 | 1:18:A:ASN:H    | 19       | 0.14          |
| (1,120) | 1:16:A:TYR:HA   | 1:16:A:TYR:HD1  | 16       | 0.14          |
| (1,120) | 1:16:A:TYR:HA   | 1:16:A:TYR:HD2  | 16       | 0.14          |
| (1,120) | 1:16:A:TYR:HA   | 1:16:A:TYR:HD1  | 17       | 0.14          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,120) | 1:16:A:TYR:HA   | 1:16:A:TYR:HD2 | 17       | 0.14          |
| (1,96)  | 1:15:A:ARG:HA   | 1:19:A:ARG:H   | 16       | 0.14          |
| (1,96)  | 1:15:A:ARG:HA   | 1:19:A:ARG:H   | 18       | 0.14          |
| (1,96)  | 1:15:A:ARG:HA   | 1:19:A:ARG:H   | 20       | 0.14          |
| (1,60)  | 1:13:A:ALA:HB1  | 1:51:A:HIS:H   | 13       | 0.14          |
| (1,60)  | 1:13:A:ALA:HB2  | 1:51:A:HIS:H   | 13       | 0.14          |
| (1,60)  | 1:13:A:ALA:HB3  | 1:51:A:HIS:H   | 13       | 0.14          |
| (1,56)  | 1:13:A:ALA:HB1  | 1:16:A:TYR:HD1 | 11       | 0.14          |
| (1,56)  | 1:13:A:ALA:HB1  | 1:16:A:TYR:HD2 | 11       | 0.14          |
| (1,56)  | 1:13:A:ALA:HB2  | 1:16:A:TYR:HD1 | 11       | 0.14          |
| (1,56)  | 1:13:A:ALA:HB2  | 1:16:A:TYR:HD2 | 11       | 0.14          |
| (1,56)  | 1:13:A:ALA:HB3  | 1:16:A:TYR:HD1 | 11       | 0.14          |
| (1,56)  | 1:13:A:ALA:HB3  | 1:16:A:TYR:HD2 | 11       | 0.14          |
| (1,56)  | 1:13:A:ALA:HB1  | 1:16:A:TYR:HD1 | 14       | 0.14          |
| (1,56)  | 1:13:A:ALA:HB1  | 1:16:A:TYR:HD2 | 14       | 0.14          |
| (1,56)  | 1:13:A:ALA:HB2  | 1:16:A:TYR:HD1 | 14       | 0.14          |
| (1,56)  | 1:13:A:ALA:HB2  | 1:16:A:TYR:HD2 | 14       | 0.14          |
| (1,56)  | 1:13:A:ALA:HB3  | 1:16:A:TYR:HD1 | 14       | 0.14          |
| (1,56)  | 1:13:A:ALA:HB3  | 1:16:A:TYR:HD2 | 14       | 0.14          |
| (1,9)   | 1:10:A:THR:HG21 | 1:53:A:ASP:HA  | 2        | 0.14          |
| (1,9)   | 1:10:A:THR:HG22 | 1:53:A:ASP:HA  | 2        | 0.14          |
| (1,9)   | 1:10:A:THR:HG23 | 1:53:A:ASP:HA  | 2        | 0.14          |
| (1,9)   | 1:10:A:THR:HG21 | 1:53:A:ASP:HA  | 3        | 0.14          |
| (1,9)   | 1:10:A:THR:HG22 | 1:53:A:ASP:HA  | 3        | 0.14          |
| (1,9)   | 1:10:A:THR:HG23 | 1:53:A:ASP:HA  | 3        | 0.14          |
| (1,9)   | 1:10:A:THR:HG21 | 1:53:A:ASP:HA  | 4        | 0.14          |
| (1,9)   | 1:10:A:THR:HG22 | 1:53:A:ASP:HA  | 4        | 0.14          |
| (1,9)   | 1:10:A:THR:HG23 | 1:53:A:ASP:HA  | 4        | 0.14          |
| (1,9)   | 1:10:A:THR:HG21 | 1:53:A:ASP:HA  | 5        | 0.14          |
| (1,9)   | 1:10:A:THR:HG22 | 1:53:A:ASP:HA  | 5        | 0.14          |
| (1,9)   | 1:10:A:THR:HG23 | 1:53:A:ASP:HA  | 5        | 0.14          |
| (1,9)   | 1:10:A:THR:HG21 | 1:53:A:ASP:HA  | 6        | 0.14          |
| (1,9)   | 1:10:A:THR:HG22 | 1:53:A:ASP:HA  | 6        | 0.14          |
| (1,9)   | 1:10:A:THR:HG23 | 1:53:A:ASP:HA  | 6        | 0.14          |
| (1,9)   | 1:10:A:THR:HG21 | 1:53:A:ASP:HA  | 7        | 0.14          |
| (1,9)   | 1:10:A:THR:HG22 | 1:53:A:ASP:HA  | 7        | 0.14          |
| (1,9)   | 1:10:A:THR:HG23 | 1:53:A:ASP:HA  | 7        | 0.14          |
| (1,9)   | 1:10:A:THR:HG21 | 1:53:A:ASP:HA  | 8        | 0.14          |
| (1,9)   | 1:10:A:THR:HG22 | 1:53:A:ASP:HA  | 8        | 0.14          |
| (1,9)   | 1:10:A:THR:HG23 | 1:53:A:ASP:HA  | 8        | 0.14          |
| (1,9)   | 1:10:A:THR:HG21 | 1:53:A:ASP:HA  | 9        | 0.14          |
| (1,9)   | 1:10:A:THR:HG22 | 1:53:A:ASP:HA  | 9        | 0.14          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (1,9)    | 1:10:A:THR:HG23 | 1:53:A:ASP:HA | 9        | 0.14          |
| (1,9)    | 1:10:A:THR:HG21 | 1:53:A:ASP:HA | 10       | 0.14          |
| (1,9)    | 1:10:A:THR:HG22 | 1:53:A:ASP:HA | 10       | 0.14          |
| (1,9)    | 1:10:A:THR:HG23 | 1:53:A:ASP:HA | 10       | 0.14          |
| (1,9)    | 1:10:A:THR:HG21 | 1:53:A:ASP:HA | 11       | 0.14          |
| (1,9)    | 1:10:A:THR:HG22 | 1:53:A:ASP:HA | 11       | 0.14          |
| (1,9)    | 1:10:A:THR:HG23 | 1:53:A:ASP:HA | 11       | 0.14          |
| (1,9)    | 1:10:A:THR:HG21 | 1:53:A:ASP:HA | 12       | 0.14          |
| (1,9)    | 1:10:A:THR:HG22 | 1:53:A:ASP:HA | 12       | 0.14          |
| (1,9)    | 1:10:A:THR:HG23 | 1:53:A:ASP:HA | 12       | 0.14          |
| (1,9)    | 1:10:A:THR:HG21 | 1:53:A:ASP:HA | 15       | 0.14          |
| (1,9)    | 1:10:A:THR:HG22 | 1:53:A:ASP:HA | 15       | 0.14          |
| (1,9)    | 1:10:A:THR:HG23 | 1:53:A:ASP:HA | 15       | 0.14          |
| (1,9)    | 1:10:A:THR:HG21 | 1:53:A:ASP:HA | 17       | 0.14          |
| (1,9)    | 1:10:A:THR:HG22 | 1:53:A:ASP:HA | 17       | 0.14          |
| (1,9)    | 1:10:A:THR:HG23 | 1:53:A:ASP:HA | 17       | 0.14          |
| (1,9)    | 1:10:A:THR:HG21 | 1:53:A:ASP:HA | 18       | 0.14          |
| (1,9)    | 1:10:A:THR:HG22 | 1:53:A:ASP:HA | 18       | 0.14          |
| (1,9)    | 1:10:A:THR:HG23 | 1:53:A:ASP:HA | 18       | 0.14          |
| (1,9)    | 1:10:A:THR:HG21 | 1:53:A:ASP:HA | 19       | 0.14          |
| (1,9)    | 1:10:A:THR:HG22 | 1:53:A:ASP:HA | 19       | 0.14          |
| (1,9)    | 1:10:A:THR:HG23 | 1:53:A:ASP:HA | 19       | 0.14          |
| (1,9)    | 1:10:A:THR:HG21 | 1:53:A:ASP:HA | 20       | 0.14          |
| (1,9)    | 1:10:A:THR:HG22 | 1:53:A:ASP:HA | 20       | 0.14          |
| (1,9)    | 1:10:A:THR:HG23 | 1:53:A:ASP:HA | 20       | 0.14          |
| (1,1328) | 1:89:A:ILE:HG21 | 1:91:A:TRP:H  | 2        | 0.13          |
| (1,1328) | 1:89:A:ILE:HG22 | 1:91:A:TRP:H  | 2        | 0.13          |
| (1,1328) | 1:89:A:ILE:HG23 | 1:91:A:TRP:H  | 2        | 0.13          |
| (1,1328) | 1:89:A:ILE:HG21 | 1:91:A:TRP:H  | 3        | 0.13          |
| (1,1328) | 1:89:A:ILE:HG22 | 1:91:A:TRP:H  | 3        | 0.13          |
| (1,1328) | 1:89:A:ILE:HG23 | 1:91:A:TRP:H  | 3        | 0.13          |
| (1,1328) | 1:89:A:ILE:HG21 | 1:91:A:TRP:H  | 5        | 0.13          |
| (1,1328) | 1:89:A:ILE:HG22 | 1:91:A:TRP:H  | 5        | 0.13          |
| (1,1328) | 1:89:A:ILE:HG23 | 1:91:A:TRP:H  | 5        | 0.13          |
| (1,1328) | 1:89:A:ILE:HG21 | 1:91:A:TRP:H  | 7        | 0.13          |
| (1,1328) | 1:89:A:ILE:HG22 | 1:91:A:TRP:H  | 7        | 0.13          |
| (1,1328) | 1:89:A:ILE:HG23 | 1:91:A:TRP:H  | 7        | 0.13          |
| (1,1328) | 1:89:A:ILE:HG21 | 1:91:A:TRP:H  | 8        | 0.13          |
| (1,1328) | 1:89:A:ILE:HG22 | 1:91:A:TRP:H  | 8        | 0.13          |
| (1,1328) | 1:89:A:ILE:HG23 | 1:91:A:TRP:H  | 8        | 0.13          |
| (1,1328) | 1:89:A:ILE:HG21 | 1:91:A:TRP:H  | 10       | 0.13          |
| (1,1328) | 1:89:A:ILE:HG22 | 1:91:A:TRP:H  | 10       | 0.13          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1328) | 1:89:A:ILE:HG23 | 1:91:A:TRP:H   | 10       | 0.13          |
| (1,1328) | 1:89:A:ILE:HG21 | 1:91:A:TRP:H   | 14       | 0.13          |
| (1,1328) | 1:89:A:ILE:HG22 | 1:91:A:TRP:H   | 14       | 0.13          |
| (1,1328) | 1:89:A:ILE:HG23 | 1:91:A:TRP:H   | 14       | 0.13          |
| (1,1328) | 1:89:A:ILE:HG21 | 1:91:A:TRP:H   | 16       | 0.13          |
| (1,1328) | 1:89:A:ILE:HG22 | 1:91:A:TRP:H   | 16       | 0.13          |
| (1,1328) | 1:89:A:ILE:HG23 | 1:91:A:TRP:H   | 16       | 0.13          |
| (1,1328) | 1:89:A:ILE:HG21 | 1:91:A:TRP:H   | 17       | 0.13          |
| (1,1328) | 1:89:A:ILE:HG22 | 1:91:A:TRP:H   | 17       | 0.13          |
| (1,1328) | 1:89:A:ILE:HG23 | 1:91:A:TRP:H   | 17       | 0.13          |
| (1,1328) | 1:89:A:ILE:HG21 | 1:91:A:TRP:H   | 18       | 0.13          |
| (1,1328) | 1:89:A:ILE:HG22 | 1:91:A:TRP:H   | 18       | 0.13          |
| (1,1328) | 1:89:A:ILE:HG23 | 1:91:A:TRP:H   | 18       | 0.13          |
| (1,1315) | 1:87:A:LEU:HG   | 1:87:A:LEU:H   | 13       | 0.13          |
| (1,1309) | 1:87:A:LEU:HB2  | 1:87:A:LEU:H   | 1        | 0.13          |
| (1,1309) | 1:87:A:LEU:HB2  | 1:87:A:LEU:H   | 7        | 0.13          |
| (1,1309) | 1:87:A:LEU:HB2  | 1:87:A:LEU:H   | 9        | 0.13          |
| (1,1309) | 1:87:A:LEU:HB2  | 1:87:A:LEU:H   | 17       | 0.13          |
| (1,1145) | 1:74:A:VAL:HB   | 1:76:A:ASP:H   | 6        | 0.13          |
| (1,1145) | 1:74:A:VAL:HB   | 1:76:A:ASP:H   | 8        | 0.13          |
| (1,1015) | 1:68:A:ALA:HA   | 1:71:A:GLN:HB2 | 2        | 0.13          |
| (1,1015) | 1:68:A:ALA:HA   | 1:71:A:GLN:HB2 | 9        | 0.13          |
| (1,1001) | 1:67:A:LEU:HB3  | 1:67:A:LEU:H   | 2        | 0.13          |
| (1,1001) | 1:67:A:LEU:HB3  | 1:67:A:LEU:H   | 9        | 0.13          |
| (1,992)  | 1:66:A:SER:H    | 1:67:A:LEU:H   | 9        | 0.13          |
| (1,992)  | 1:66:A:SER:H    | 1:67:A:LEU:H   | 16       | 0.13          |
| (1,992)  | 1:66:A:SER:H    | 1:67:A:LEU:H   | 17       | 0.13          |
| (1,954)  | 1:64:A:GLU:HA   | 1:67:A:LEU:HG  | 4        | 0.13          |
| (1,954)  | 1:64:A:GLU:HA   | 1:67:A:LEU:HG  | 12       | 0.13          |
| (1,954)  | 1:64:A:GLU:HA   | 1:67:A:LEU:HG  | 14       | 0.13          |
| (1,954)  | 1:64:A:GLU:HA   | 1:67:A:LEU:HG  | 19       | 0.13          |
| (1,942)  | 1:63:A:ASP:H    | 1:67:A:LEU:HB3 | 1        | 0.13          |
| (1,942)  | 1:63:A:ASP:H    | 1:67:A:LEU:HB3 | 3        | 0.13          |
| (1,942)  | 1:63:A:ASP:H    | 1:67:A:LEU:HB3 | 5        | 0.13          |
| (1,942)  | 1:63:A:ASP:H    | 1:67:A:LEU:HB3 | 6        | 0.13          |
| (1,942)  | 1:63:A:ASP:H    | 1:67:A:LEU:HB3 | 7        | 0.13          |
| (1,942)  | 1:63:A:ASP:H    | 1:67:A:LEU:HB3 | 9        | 0.13          |
| (1,942)  | 1:63:A:ASP:H    | 1:67:A:LEU:HB3 | 10       | 0.13          |
| (1,942)  | 1:63:A:ASP:H    | 1:67:A:LEU:HB3 | 11       | 0.13          |
| (1,942)  | 1:63:A:ASP:H    | 1:67:A:LEU:HB3 | 14       | 0.13          |
| (1,942)  | 1:63:A:ASP:H    | 1:67:A:LEU:HB3 | 17       | 0.13          |
| (1,942)  | 1:63:A:ASP:H    | 1:67:A:LEU:HB3 | 18       | 0.13          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,938) | 1:63:A:ASP:H   | 1:66:A:SER:HA  | 2        | 0.13          |
| (1,938) | 1:63:A:ASP:H   | 1:66:A:SER:HA  | 7        | 0.13          |
| (1,938) | 1:63:A:ASP:H   | 1:66:A:SER:HA  | 9        | 0.13          |
| (1,938) | 1:63:A:ASP:H   | 1:66:A:SER:HA  | 12       | 0.13          |
| (1,922) | 1:62:A:PRO:HB3 | 1:63:A:ASP:H   | 3        | 0.13          |
| (1,922) | 1:62:A:PRO:HB3 | 1:63:A:ASP:H   | 4        | 0.13          |
| (1,922) | 1:62:A:PRO:HB3 | 1:63:A:ASP:H   | 6        | 0.13          |
| (1,922) | 1:62:A:PRO:HB3 | 1:63:A:ASP:H   | 7        | 0.13          |
| (1,922) | 1:62:A:PRO:HB3 | 1:63:A:ASP:H   | 8        | 0.13          |
| (1,922) | 1:62:A:PRO:HB3 | 1:63:A:ASP:H   | 10       | 0.13          |
| (1,922) | 1:62:A:PRO:HB3 | 1:63:A:ASP:H   | 15       | 0.13          |
| (1,922) | 1:62:A:PRO:HB3 | 1:63:A:ASP:H   | 16       | 0.13          |
| (1,914) | 1:61:A:SER:HB2 | 1:67:A:LEU:HA  | 5        | 0.13          |
| (1,914) | 1:61:A:SER:HB3 | 1:67:A:LEU:HA  | 5        | 0.13          |
| (1,914) | 1:61:A:SER:HB2 | 1:67:A:LEU:HA  | 6        | 0.13          |
| (1,914) | 1:61:A:SER:HB3 | 1:67:A:LEU:HA  | 6        | 0.13          |
| (1,914) | 1:61:A:SER:HB2 | 1:67:A:LEU:HA  | 11       | 0.13          |
| (1,914) | 1:61:A:SER:HB3 | 1:67:A:LEU:HA  | 11       | 0.13          |
| (1,914) | 1:61:A:SER:HB2 | 1:67:A:LEU:HA  | 12       | 0.13          |
| (1,914) | 1:61:A:SER:HB3 | 1:67:A:LEU:HA  | 12       | 0.13          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG21 | 2        | 0.13          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG22 | 2        | 0.13          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG23 | 2        | 0.13          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG21 | 4        | 0.13          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG22 | 4        | 0.13          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG23 | 4        | 0.13          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG21 | 5        | 0.13          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG22 | 5        | 0.13          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG23 | 5        | 0.13          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG21 | 6        | 0.13          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG22 | 6        | 0.13          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG23 | 6        | 0.13          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG21 | 7        | 0.13          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG22 | 7        | 0.13          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG23 | 7        | 0.13          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG21 | 9        | 0.13          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG22 | 9        | 0.13          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG23 | 9        | 0.13          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG21 | 10       | 0.13          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG22 | 10       | 0.13          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG23 | 10       | 0.13          |
| (1,878) | 1:5:A:THR:HA   | 1:5:A:THR:HG21 | 11       | 0.13          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,878) | 1:5:A:THR:HA  | 1:5:A:THR:HG22 | 11       | 0.13          |
| (1,878) | 1:5:A:THR:HA  | 1:5:A:THR:HG23 | 11       | 0.13          |
| (1,878) | 1:5:A:THR:HA  | 1:5:A:THR:HG21 | 14       | 0.13          |
| (1,878) | 1:5:A:THR:HA  | 1:5:A:THR:HG22 | 14       | 0.13          |
| (1,878) | 1:5:A:THR:HA  | 1:5:A:THR:HG23 | 14       | 0.13          |
| (1,878) | 1:5:A:THR:HA  | 1:5:A:THR:HG21 | 16       | 0.13          |
| (1,878) | 1:5:A:THR:HA  | 1:5:A:THR:HG22 | 16       | 0.13          |
| (1,878) | 1:5:A:THR:HA  | 1:5:A:THR:HG23 | 16       | 0.13          |
| (1,878) | 1:5:A:THR:HA  | 1:5:A:THR:HG21 | 17       | 0.13          |
| (1,878) | 1:5:A:THR:HA  | 1:5:A:THR:HG22 | 17       | 0.13          |
| (1,878) | 1:5:A:THR:HA  | 1:5:A:THR:HG23 | 17       | 0.13          |
| (1,878) | 1:5:A:THR:HA  | 1:5:A:THR:HG21 | 19       | 0.13          |
| (1,878) | 1:5:A:THR:HA  | 1:5:A:THR:HG22 | 19       | 0.13          |
| (1,878) | 1:5:A:THR:HA  | 1:5:A:THR:HG23 | 19       | 0.13          |
| (1,832) | 1:57:A:MET:HA | 1:58:A:ILE:H   | 3        | 0.13          |
| (1,832) | 1:57:A:MET:HA | 1:58:A:ILE:H   | 6        | 0.13          |
| (1,832) | 1:57:A:MET:HA | 1:58:A:ILE:H   | 8        | 0.13          |
| (1,832) | 1:57:A:MET:HA | 1:58:A:ILE:H   | 11       | 0.13          |
| (1,832) | 1:57:A:MET:HA | 1:58:A:ILE:H   | 12       | 0.13          |
| (1,832) | 1:57:A:MET:HA | 1:58:A:ILE:H   | 14       | 0.13          |
| (1,832) | 1:57:A:MET:HA | 1:58:A:ILE:H   | 18       | 0.13          |
| (1,800) | 1:54:A:HIS:HA | 1:55:A:VAL:H   | 2        | 0.13          |
| (1,800) | 1:54:A:HIS:HA | 1:55:A:VAL:H   | 3        | 0.13          |
| (1,800) | 1:54:A:HIS:HA | 1:55:A:VAL:H   | 6        | 0.13          |
| (1,800) | 1:54:A:HIS:HA | 1:55:A:VAL:H   | 7        | 0.13          |
| (1,800) | 1:54:A:HIS:HA | 1:55:A:VAL:H   | 8        | 0.13          |
| (1,800) | 1:54:A:HIS:HA | 1:55:A:VAL:H   | 11       | 0.13          |
| (1,800) | 1:54:A:HIS:HA | 1:55:A:VAL:H   | 12       | 0.13          |
| (1,800) | 1:54:A:HIS:HA | 1:55:A:VAL:H   | 15       | 0.13          |
| (1,800) | 1:54:A:HIS:HA | 1:55:A:VAL:H   | 16       | 0.13          |
| (1,800) | 1:54:A:HIS:HA | 1:55:A:VAL:H   | 18       | 0.13          |
| (1,744) | 1:4:A:SER:HB2 | 1:93:A:PRO:HB2 | 5        | 0.13          |
| (1,744) | 1:4:A:SER:HB3 | 1:93:A:PRO:HB2 | 5        | 0.13          |
| (1,744) | 1:4:A:SER:HB2 | 1:93:A:PRO:HB2 | 6        | 0.13          |
| (1,744) | 1:4:A:SER:HB3 | 1:93:A:PRO:HB2 | 6        | 0.13          |
| (1,744) | 1:4:A:SER:HB2 | 1:93:A:PRO:HB2 | 8        | 0.13          |
| (1,744) | 1:4:A:SER:HB3 | 1:93:A:PRO:HB2 | 8        | 0.13          |
| (1,744) | 1:4:A:SER:HB2 | 1:93:A:PRO:HB2 | 10       | 0.13          |
| (1,744) | 1:4:A:SER:HB3 | 1:93:A:PRO:HB2 | 10       | 0.13          |
| (1,744) | 1:4:A:SER:HB2 | 1:93:A:PRO:HB2 | 11       | 0.13          |
| (1,744) | 1:4:A:SER:HB3 | 1:93:A:PRO:HB2 | 11       | 0.13          |
| (1,744) | 1:4:A:SER:HB2 | 1:93:A:PRO:HB2 | 12       | 0.13          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,744) | 1:4:A:SER:HB3  | 1:93:A:PRO:HB2 | 12       | 0.13          |
| (1,744) | 1:4:A:SER:HB2  | 1:93:A:PRO:HB2 | 14       | 0.13          |
| (1,744) | 1:4:A:SER:HB3  | 1:93:A:PRO:HB2 | 14       | 0.13          |
| (1,744) | 1:4:A:SER:HB2  | 1:93:A:PRO:HB2 | 15       | 0.13          |
| (1,744) | 1:4:A:SER:HB3  | 1:93:A:PRO:HB2 | 15       | 0.13          |
| (1,744) | 1:4:A:SER:HB2  | 1:93:A:PRO:HB2 | 17       | 0.13          |
| (1,744) | 1:4:A:SER:HB3  | 1:93:A:PRO:HB2 | 17       | 0.13          |
| (1,744) | 1:4:A:SER:HB2  | 1:93:A:PRO:HB2 | 18       | 0.13          |
| (1,744) | 1:4:A:SER:HB3  | 1:93:A:PRO:HB2 | 18       | 0.13          |
| (1,744) | 1:4:A:SER:HB2  | 1:93:A:PRO:HB2 | 20       | 0.13          |
| (1,744) | 1:4:A:SER:HB3  | 1:93:A:PRO:HB2 | 20       | 0.13          |
| (1,726) | 1:49:A:LEU:H   | 1:57:A:MET:HG2 | 3        | 0.13          |
| (1,726) | 1:49:A:LEU:H   | 1:57:A:MET:HG2 | 8        | 0.13          |
| (1,726) | 1:49:A:LEU:H   | 1:57:A:MET:HG2 | 10       | 0.13          |
| (1,726) | 1:49:A:LEU:H   | 1:57:A:MET:HG2 | 11       | 0.13          |
| (1,704) | 1:48:A:LEU:HB2 | 1:48:A:LEU:H   | 8        | 0.13          |
| (1,704) | 1:48:A:LEU:HB3 | 1:48:A:LEU:H   | 8        | 0.13          |
| (1,704) | 1:48:A:LEU:HB2 | 1:48:A:LEU:H   | 9        | 0.13          |
| (1,704) | 1:48:A:LEU:HB3 | 1:48:A:LEU:H   | 9        | 0.13          |
| (1,704) | 1:48:A:LEU:HB2 | 1:48:A:LEU:H   | 15       | 0.13          |
| (1,704) | 1:48:A:LEU:HB3 | 1:48:A:LEU:H   | 15       | 0.13          |
| (1,704) | 1:48:A:LEU:HB2 | 1:48:A:LEU:H   | 18       | 0.13          |
| (1,704) | 1:48:A:LEU:HB3 | 1:48:A:LEU:H   | 18       | 0.13          |
| (1,673) | 1:45:A:ASN:H   | 1:70:A:MET:HB3 | 10       | 0.13          |
| (1,673) | 1:45:A:ASN:H   | 1:70:A:MET:HB3 | 13       | 0.13          |
| (1,651) | 1:44:A:SER:HB3 | 1:61:A:SER:HA  | 4        | 0.13          |
| (1,589) | 1:3:A:ARG:HB2  | 1:3:A:ARG:H    | 4        | 0.13          |
| (1,589) | 1:3:A:ARG:HB3  | 1:3:A:ARG:H    | 4        | 0.13          |
| (1,589) | 1:3:A:ARG:HB2  | 1:3:A:ARG:H    | 5        | 0.13          |
| (1,589) | 1:3:A:ARG:HB3  | 1:3:A:ARG:H    | 5        | 0.13          |
| (1,589) | 1:3:A:ARG:HB2  | 1:3:A:ARG:H    | 10       | 0.13          |
| (1,589) | 1:3:A:ARG:HB3  | 1:3:A:ARG:H    | 10       | 0.13          |
| (1,589) | 1:3:A:ARG:HB2  | 1:3:A:ARG:H    | 11       | 0.13          |
| (1,589) | 1:3:A:ARG:HB3  | 1:3:A:ARG:H    | 11       | 0.13          |
| (1,589) | 1:3:A:ARG:HB2  | 1:3:A:ARG:H    | 12       | 0.13          |
| (1,589) | 1:3:A:ARG:HB3  | 1:3:A:ARG:H    | 12       | 0.13          |
| (1,589) | 1:3:A:ARG:HB2  | 1:3:A:ARG:H    | 13       | 0.13          |
| (1,589) | 1:3:A:ARG:HB3  | 1:3:A:ARG:H    | 13       | 0.13          |
| (1,589) | 1:3:A:ARG:HB2  | 1:3:A:ARG:H    | 14       | 0.13          |
| (1,589) | 1:3:A:ARG:HB3  | 1:3:A:ARG:H    | 14       | 0.13          |
| (1,589) | 1:3:A:ARG:HB2  | 1:3:A:ARG:H    | 16       | 0.13          |
| (1,589) | 1:3:A:ARG:HB3  | 1:3:A:ARG:H    | 16       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,589) | 1:3:A:ARG:HB2   | 1:3:A:ARG:H     | 17       | 0.13          |
| (1,589) | 1:3:A:ARG:HB3   | 1:3:A:ARG:H     | 17       | 0.13          |
| (1,589) | 1:3:A:ARG:HB2   | 1:3:A:ARG:H     | 19       | 0.13          |
| (1,589) | 1:3:A:ARG:HB3   | 1:3:A:ARG:H     | 19       | 0.13          |
| (1,539) | 1:38:A:PHE:HD1  | 1:48:A:LEU:H    | 2        | 0.13          |
| (1,539) | 1:38:A:PHE:HD2  | 1:48:A:LEU:H    | 2        | 0.13          |
| (1,521) | 1:38:A:PHE:HA   | 1:46:A:CYS:H    | 14       | 0.13          |
| (1,521) | 1:38:A:PHE:HA   | 1:46:A:CYS:H    | 19       | 0.13          |
| (1,454) | 1:33:A:THR:HA   | 1:33:A:THR:H    | 1        | 0.13          |
| (1,454) | 1:33:A:THR:HA   | 1:33:A:THR:H    | 2        | 0.13          |
| (1,454) | 1:33:A:THR:HA   | 1:33:A:THR:H    | 3        | 0.13          |
| (1,454) | 1:33:A:THR:HA   | 1:33:A:THR:H    | 4        | 0.13          |
| (1,454) | 1:33:A:THR:HA   | 1:33:A:THR:H    | 5        | 0.13          |
| (1,454) | 1:33:A:THR:HA   | 1:33:A:THR:H    | 6        | 0.13          |
| (1,454) | 1:33:A:THR:HA   | 1:33:A:THR:H    | 7        | 0.13          |
| (1,454) | 1:33:A:THR:HA   | 1:33:A:THR:H    | 8        | 0.13          |
| (1,454) | 1:33:A:THR:HA   | 1:33:A:THR:H    | 9        | 0.13          |
| (1,454) | 1:33:A:THR:HA   | 1:33:A:THR:H    | 10       | 0.13          |
| (1,454) | 1:33:A:THR:HA   | 1:33:A:THR:H    | 11       | 0.13          |
| (1,454) | 1:33:A:THR:HA   | 1:33:A:THR:H    | 12       | 0.13          |
| (1,454) | 1:33:A:THR:HA   | 1:33:A:THR:H    | 13       | 0.13          |
| (1,454) | 1:33:A:THR:HA   | 1:33:A:THR:H    | 14       | 0.13          |
| (1,454) | 1:33:A:THR:HA   | 1:33:A:THR:H    | 15       | 0.13          |
| (1,454) | 1:33:A:THR:HA   | 1:33:A:THR:H    | 16       | 0.13          |
| (1,454) | 1:33:A:THR:HA   | 1:33:A:THR:H    | 17       | 0.13          |
| (1,454) | 1:33:A:THR:HA   | 1:33:A:THR:H    | 18       | 0.13          |
| (1,454) | 1:33:A:THR:HA   | 1:33:A:THR:H    | 19       | 0.13          |
| (1,454) | 1:33:A:THR:HA   | 1:33:A:THR:H    | 20       | 0.13          |
| (1,437) | 1:32:A:LEU:HB3  | 1:32:A:LEU:H    | 11       | 0.13          |
| (1,394) | 1:2:A:PHE:H     | 1:62:A:PRO:HD2  | 4        | 0.13          |
| (1,394) | 1:2:A:PHE:H     | 1:62:A:PRO:HD3  | 4        | 0.13          |
| (1,394) | 1:2:A:PHE:H     | 1:62:A:PRO:HD2  | 7        | 0.13          |
| (1,394) | 1:2:A:PHE:H     | 1:62:A:PRO:HD3  | 7        | 0.13          |
| (1,295) | 1:24:A:TRP:H    | 1:39:A:ILE:HG21 | 20       | 0.13          |
| (1,295) | 1:24:A:TRP:H    | 1:39:A:ILE:HG22 | 20       | 0.13          |
| (1,295) | 1:24:A:TRP:H    | 1:39:A:ILE:HG23 | 20       | 0.13          |
| (1,194) | 1:19:A:ARG:H    | 1:20:A:LEU:HG   | 16       | 0.13          |
| (1,151) | 1:17:A:VAL:HG11 | 1:18:A:ASN:H    | 3        | 0.13          |
| (1,151) | 1:17:A:VAL:HG12 | 1:18:A:ASN:H    | 3        | 0.13          |
| (1,151) | 1:17:A:VAL:HG13 | 1:18:A:ASN:H    | 3        | 0.13          |
| (1,151) | 1:17:A:VAL:HG11 | 1:18:A:ASN:H    | 8        | 0.13          |
| (1,151) | 1:17:A:VAL:HG12 | 1:18:A:ASN:H    | 8        | 0.13          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,151)  | 1:17:A:VAL:HG13 | 1:18:A:ASN:H   | 8        | 0.13          |
| (1,116)  | 1:15:A:ARG:HG2  | 1:16:A:TYR:H   | 2        | 0.13          |
| (1,116)  | 1:15:A:ARG:HG3  | 1:16:A:TYR:H   | 2        | 0.13          |
| (1,116)  | 1:15:A:ARG:HG2  | 1:16:A:TYR:H   | 13       | 0.13          |
| (1,116)  | 1:15:A:ARG:HG3  | 1:16:A:TYR:H   | 13       | 0.13          |
| (1,113)  | 1:15:A:ARG:HD2  | 1:20:A:LEU:H   | 14       | 0.13          |
| (1,113)  | 1:15:A:ARG:HD3  | 1:20:A:LEU:H   | 14       | 0.13          |
| (1,96)   | 1:15:A:ARG:HA   | 1:19:A:ARG:H   | 4        | 0.13          |
| (1,85)   | 1:14:A:ALA:HB1  | 1:50:A:ALA:HA  | 13       | 0.13          |
| (1,85)   | 1:14:A:ALA:HB2  | 1:50:A:ALA:HA  | 13       | 0.13          |
| (1,85)   | 1:14:A:ALA:HB3  | 1:50:A:ALA:HA  | 13       | 0.13          |
| (1,56)   | 1:13:A:ALA:HB1  | 1:16:A:TYR:HD1 | 16       | 0.13          |
| (1,56)   | 1:13:A:ALA:HB1  | 1:16:A:TYR:HD2 | 16       | 0.13          |
| (1,56)   | 1:13:A:ALA:HB2  | 1:16:A:TYR:HD1 | 16       | 0.13          |
| (1,56)   | 1:13:A:ALA:HB2  | 1:16:A:TYR:HD2 | 16       | 0.13          |
| (1,56)   | 1:13:A:ALA:HB3  | 1:16:A:TYR:HD1 | 16       | 0.13          |
| (1,56)   | 1:13:A:ALA:HB3  | 1:16:A:TYR:HD2 | 16       | 0.13          |
| (1,9)    | 1:10:A:THR:HG21 | 1:53:A:ASP:HA  | 1        | 0.13          |
| (1,9)    | 1:10:A:THR:HG22 | 1:53:A:ASP:HA  | 1        | 0.13          |
| (1,9)    | 1:10:A:THR:HG23 | 1:53:A:ASP:HA  | 1        | 0.13          |
| (1,5)    | 1:10:A:THR:HG21 | 1:13:A:ALA:HA  | 13       | 0.13          |
| (1,5)    | 1:10:A:THR:HG22 | 1:13:A:ALA:HA  | 13       | 0.13          |
| (1,5)    | 1:10:A:THR:HG23 | 1:13:A:ALA:HA  | 13       | 0.13          |
| (1,5)    | 1:10:A:THR:HG21 | 1:13:A:ALA:HA  | 14       | 0.13          |
| (1,5)    | 1:10:A:THR:HG22 | 1:13:A:ALA:HA  | 14       | 0.13          |
| (1,5)    | 1:10:A:THR:HG23 | 1:13:A:ALA:HA  | 14       | 0.13          |
| (1,5)    | 1:10:A:THR:HG21 | 1:13:A:ALA:HA  | 16       | 0.13          |
| (1,5)    | 1:10:A:THR:HG22 | 1:13:A:ALA:HA  | 16       | 0.13          |
| (1,5)    | 1:10:A:THR:HG23 | 1:13:A:ALA:HA  | 16       | 0.13          |
| (1,1342) | 1:90:A:ALA:HB1  | 1:90:A:ALA:H   | 1        | 0.12          |
| (1,1342) | 1:90:A:ALA:HB2  | 1:90:A:ALA:H   | 1        | 0.12          |
| (1,1342) | 1:90:A:ALA:HB3  | 1:90:A:ALA:H   | 1        | 0.12          |
| (1,1342) | 1:90:A:ALA:HB1  | 1:90:A:ALA:H   | 16       | 0.12          |
| (1,1342) | 1:90:A:ALA:HB2  | 1:90:A:ALA:H   | 16       | 0.12          |
| (1,1342) | 1:90:A:ALA:HB3  | 1:90:A:ALA:H   | 16       | 0.12          |
| (1,1342) | 1:90:A:ALA:HB1  | 1:90:A:ALA:H   | 17       | 0.12          |
| (1,1342) | 1:90:A:ALA:HB2  | 1:90:A:ALA:H   | 17       | 0.12          |
| (1,1342) | 1:90:A:ALA:HB3  | 1:90:A:ALA:H   | 17       | 0.12          |
| (1,1328) | 1:89:A:ILE:HG21 | 1:91:A:TRP:H   | 1        | 0.12          |
| (1,1328) | 1:89:A:ILE:HG22 | 1:91:A:TRP:H   | 1        | 0.12          |
| (1,1328) | 1:89:A:ILE:HG23 | 1:91:A:TRP:H   | 1        | 0.12          |
| (1,1328) | 1:89:A:ILE:HG21 | 1:91:A:TRP:H   | 4        | 0.12          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (1,1328) | 1:89:A:ILE:HG22 | 1:91:A:TRP:H  | 4        | 0.12          |
| (1,1328) | 1:89:A:ILE:HG23 | 1:91:A:TRP:H  | 4        | 0.12          |
| (1,1328) | 1:89:A:ILE:HG21 | 1:91:A:TRP:H  | 6        | 0.12          |
| (1,1328) | 1:89:A:ILE:HG22 | 1:91:A:TRP:H  | 6        | 0.12          |
| (1,1328) | 1:89:A:ILE:HG23 | 1:91:A:TRP:H  | 6        | 0.12          |
| (1,1328) | 1:89:A:ILE:HG21 | 1:91:A:TRP:H  | 9        | 0.12          |
| (1,1328) | 1:89:A:ILE:HG22 | 1:91:A:TRP:H  | 9        | 0.12          |
| (1,1328) | 1:89:A:ILE:HG23 | 1:91:A:TRP:H  | 9        | 0.12          |
| (1,1309) | 1:87:A:LEU:HB2  | 1:87:A:LEU:H  | 3        | 0.12          |
| (1,1309) | 1:87:A:LEU:HB2  | 1:87:A:LEU:H  | 15       | 0.12          |
| (1,1309) | 1:87:A:LEU:HB2  | 1:87:A:LEU:H  | 16       | 0.12          |
| (1,1309) | 1:87:A:LEU:HB2  | 1:87:A:LEU:H  | 18       | 0.12          |
| (1,1276) | 1:80:A:ARG:HG2  | 1:81:A:MET:H  | 20       | 0.12          |
| (1,1263) | 1:7:A:HIS:HD2   | 1:9:A:ARG:HG3 | 1        | 0.12          |
| (1,1263) | 1:7:A:HIS:HD1   | 1:9:A:ARG:HG3 | 13       | 0.12          |
| (1,1145) | 1:74:A:VAL:HB   | 1:76:A:ASP:H  | 1        | 0.12          |
| (1,1145) | 1:74:A:VAL:HB   | 1:76:A:ASP:H  | 2        | 0.12          |
| (1,1145) | 1:74:A:VAL:HB   | 1:76:A:ASP:H  | 3        | 0.12          |
| (1,1145) | 1:74:A:VAL:HB   | 1:76:A:ASP:H  | 9        | 0.12          |
| (1,1145) | 1:74:A:VAL:HB   | 1:76:A:ASP:H  | 10       | 0.12          |
| (1,1145) | 1:74:A:VAL:HB   | 1:76:A:ASP:H  | 14       | 0.12          |
| (1,1145) | 1:74:A:VAL:HB   | 1:76:A:ASP:H  | 15       | 0.12          |
| (1,1145) | 1:74:A:VAL:HB   | 1:76:A:ASP:H  | 16       | 0.12          |
| (1,1145) | 1:74:A:VAL:HB   | 1:76:A:ASP:H  | 17       | 0.12          |
| (1,1145) | 1:74:A:VAL:HB   | 1:76:A:ASP:H  | 18       | 0.12          |
| (1,992)  | 1:66:A:SER:H    | 1:67:A:LEU:H  | 1        | 0.12          |
| (1,992)  | 1:66:A:SER:H    | 1:67:A:LEU:H  | 2        | 0.12          |
| (1,992)  | 1:66:A:SER:H    | 1:67:A:LEU:H  | 3        | 0.12          |
| (1,992)  | 1:66:A:SER:H    | 1:67:A:LEU:H  | 4        | 0.12          |
| (1,992)  | 1:66:A:SER:H    | 1:67:A:LEU:H  | 5        | 0.12          |
| (1,992)  | 1:66:A:SER:H    | 1:67:A:LEU:H  | 6        | 0.12          |
| (1,992)  | 1:66:A:SER:H    | 1:67:A:LEU:H  | 8        | 0.12          |
| (1,992)  | 1:66:A:SER:H    | 1:67:A:LEU:H  | 10       | 0.12          |
| (1,992)  | 1:66:A:SER:H    | 1:67:A:LEU:H  | 11       | 0.12          |
| (1,992)  | 1:66:A:SER:H    | 1:67:A:LEU:H  | 13       | 0.12          |
| (1,992)  | 1:66:A:SER:H    | 1:67:A:LEU:H  | 14       | 0.12          |
| (1,992)  | 1:66:A:SER:H    | 1:67:A:LEU:H  | 15       | 0.12          |
| (1,992)  | 1:66:A:SER:H    | 1:67:A:LEU:H  | 18       | 0.12          |
| (1,992)  | 1:66:A:SER:H    | 1:67:A:LEU:H  | 20       | 0.12          |
| (1,969)  | 1:64:A:GLU:H    | 1:65:A:ASP:H  | 14       | 0.12          |
| (1,969)  | 1:64:A:GLU:H    | 1:65:A:ASP:H  | 19       | 0.12          |
| (1,954)  | 1:64:A:GLU:HA   | 1:67:A:LEU:HG | 3        | 0.12          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,954) | 1:64:A:GLU:HA  | 1:67:A:LEU:HG  | 5        | 0.12          |
| (1,954) | 1:64:A:GLU:HA  | 1:67:A:LEU:HG  | 11       | 0.12          |
| (1,954) | 1:64:A:GLU:HA  | 1:67:A:LEU:HG  | 13       | 0.12          |
| (1,954) | 1:64:A:GLU:HA  | 1:67:A:LEU:HG  | 16       | 0.12          |
| (1,954) | 1:64:A:GLU:HA  | 1:67:A:LEU:HG  | 17       | 0.12          |
| (1,942) | 1:63:A:ASP:H   | 1:67:A:LEU:HB3 | 4        | 0.12          |
| (1,942) | 1:63:A:ASP:H   | 1:67:A:LEU:HB3 | 13       | 0.12          |
| (1,942) | 1:63:A:ASP:H   | 1:67:A:LEU:HB3 | 15       | 0.12          |
| (1,942) | 1:63:A:ASP:H   | 1:67:A:LEU:HB3 | 16       | 0.12          |
| (1,938) | 1:63:A:ASP:H   | 1:66:A:SER:HA  | 1        | 0.12          |
| (1,938) | 1:63:A:ASP:H   | 1:66:A:SER:HA  | 3        | 0.12          |
| (1,938) | 1:63:A:ASP:H   | 1:66:A:SER:HA  | 4        | 0.12          |
| (1,938) | 1:63:A:ASP:H   | 1:66:A:SER:HA  | 6        | 0.12          |
| (1,938) | 1:63:A:ASP:H   | 1:66:A:SER:HA  | 11       | 0.12          |
| (1,938) | 1:63:A:ASP:H   | 1:66:A:SER:HA  | 15       | 0.12          |
| (1,938) | 1:63:A:ASP:H   | 1:66:A:SER:HA  | 17       | 0.12          |
| (1,922) | 1:62:A:PRO:HB3 | 1:63:A:ASP:H   | 14       | 0.12          |
| (1,922) | 1:62:A:PRO:HB3 | 1:63:A:ASP:H   | 19       | 0.12          |
| (1,914) | 1:61:A:SER:HB2 | 1:67:A:LEU:HA  | 3        | 0.12          |
| (1,914) | 1:61:A:SER:HB3 | 1:67:A:LEU:HA  | 3        | 0.12          |
| (1,914) | 1:61:A:SER:HB2 | 1:67:A:LEU:HA  | 8        | 0.12          |
| (1,914) | 1:61:A:SER:HB3 | 1:67:A:LEU:HA  | 8        | 0.12          |
| (1,914) | 1:61:A:SER:HB2 | 1:67:A:LEU:HA  | 13       | 0.12          |
| (1,914) | 1:61:A:SER:HB3 | 1:67:A:LEU:HA  | 13       | 0.12          |
| (1,914) | 1:61:A:SER:HB2 | 1:67:A:LEU:HA  | 16       | 0.12          |
| (1,914) | 1:61:A:SER:HB3 | 1:67:A:LEU:HA  | 16       | 0.12          |
| (1,911) | 1:61:A:SER:HB2 | 1:62:A:PRO:HD2 | 4        | 0.12          |
| (1,911) | 1:61:A:SER:HB2 | 1:62:A:PRO:HD3 | 4        | 0.12          |
| (1,911) | 1:61:A:SER:HB3 | 1:62:A:PRO:HD2 | 4        | 0.12          |
| (1,911) | 1:61:A:SER:HB3 | 1:62:A:PRO:HD3 | 4        | 0.12          |
| (1,911) | 1:61:A:SER:HB2 | 1:62:A:PRO:HD2 | 7        | 0.12          |
| (1,911) | 1:61:A:SER:HB2 | 1:62:A:PRO:HD3 | 7        | 0.12          |
| (1,911) | 1:61:A:SER:HB3 | 1:62:A:PRO:HD2 | 7        | 0.12          |
| (1,911) | 1:61:A:SER:HB3 | 1:62:A:PRO:HD3 | 7        | 0.12          |
| (1,832) | 1:57:A:MET:HA  | 1:58:A:ILE:H   | 1        | 0.12          |
| (1,832) | 1:57:A:MET:HA  | 1:58:A:ILE:H   | 2        | 0.12          |
| (1,832) | 1:57:A:MET:HA  | 1:58:A:ILE:H   | 4        | 0.12          |
| (1,832) | 1:57:A:MET:HA  | 1:58:A:ILE:H   | 5        | 0.12          |
| (1,832) | 1:57:A:MET:HA  | 1:58:A:ILE:H   | 7        | 0.12          |
| (1,832) | 1:57:A:MET:HA  | 1:58:A:ILE:H   | 9        | 0.12          |
| (1,832) | 1:57:A:MET:HA  | 1:58:A:ILE:H   | 10       | 0.12          |
| (1,832) | 1:57:A:MET:HA  | 1:58:A:ILE:H   | 13       | 0.12          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,832) | 1:57:A:MET:HA  | 1:58:A:ILE:H    | 15       | 0.12          |
| (1,832) | 1:57:A:MET:HA  | 1:58:A:ILE:H    | 16       | 0.12          |
| (1,832) | 1:57:A:MET:HA  | 1:58:A:ILE:H    | 17       | 0.12          |
| (1,832) | 1:57:A:MET:HA  | 1:58:A:ILE:H    | 19       | 0.12          |
| (1,808) | 1:54:A:HIS:HD1 | 1:56:A:LEU:HD13 | 10       | 0.12          |
| (1,800) | 1:54:A:HIS:HA  | 1:55:A:VAL:H    | 1        | 0.12          |
| (1,800) | 1:54:A:HIS:HA  | 1:55:A:VAL:H    | 4        | 0.12          |
| (1,800) | 1:54:A:HIS:HA  | 1:55:A:VAL:H    | 5        | 0.12          |
| (1,800) | 1:54:A:HIS:HA  | 1:55:A:VAL:H    | 9        | 0.12          |
| (1,800) | 1:54:A:HIS:HA  | 1:55:A:VAL:H    | 10       | 0.12          |
| (1,800) | 1:54:A:HIS:HA  | 1:55:A:VAL:H    | 14       | 0.12          |
| (1,800) | 1:54:A:HIS:HA  | 1:55:A:VAL:H    | 17       | 0.12          |
| (1,800) | 1:54:A:HIS:HA  | 1:55:A:VAL:H    | 19       | 0.12          |
| (1,800) | 1:54:A:HIS:HA  | 1:55:A:VAL:H    | 20       | 0.12          |
| (1,774) | 1:51:A:HIS:H   | 1:52:A:PRO:HD2  | 10       | 0.12          |
| (1,773) | 1:51:A:HIS:H   | 1:52:A:PRO:HD3  | 7        | 0.12          |
| (1,773) | 1:51:A:HIS:H   | 1:52:A:PRO:HD3  | 11       | 0.12          |
| (1,773) | 1:51:A:HIS:H   | 1:52:A:PRO:HD3  | 12       | 0.12          |
| (1,773) | 1:51:A:HIS:H   | 1:52:A:PRO:HD3  | 14       | 0.12          |
| (1,773) | 1:51:A:HIS:H   | 1:52:A:PRO:HD3  | 15       | 0.12          |
| (1,773) | 1:51:A:HIS:H   | 1:52:A:PRO:HD3  | 18       | 0.12          |
| (1,744) | 1:4:A:SER:HB2  | 1:93:A:PRO:HB2  | 4        | 0.12          |
| (1,744) | 1:4:A:SER:HB3  | 1:93:A:PRO:HB2  | 4        | 0.12          |
| (1,744) | 1:4:A:SER:HB2  | 1:93:A:PRO:HB2  | 16       | 0.12          |
| (1,744) | 1:4:A:SER:HB3  | 1:93:A:PRO:HB2  | 16       | 0.12          |
| (1,744) | 1:4:A:SER:HB2  | 1:93:A:PRO:HB2  | 19       | 0.12          |
| (1,744) | 1:4:A:SER:HB3  | 1:93:A:PRO:HB2  | 19       | 0.12          |
| (1,739) | 1:4:A:SER:HB2  | 1:59:A:LEU:HB2  | 2        | 0.12          |
| (1,739) | 1:4:A:SER:HB2  | 1:59:A:LEU:HB3  | 2        | 0.12          |
| (1,739) | 1:4:A:SER:HB3  | 1:59:A:LEU:HB2  | 2        | 0.12          |
| (1,739) | 1:4:A:SER:HB3  | 1:59:A:LEU:HB3  | 2        | 0.12          |
| (1,739) | 1:4:A:SER:HB2  | 1:59:A:LEU:HB2  | 9        | 0.12          |
| (1,739) | 1:4:A:SER:HB2  | 1:59:A:LEU:HB3  | 9        | 0.12          |
| (1,739) | 1:4:A:SER:HB3  | 1:59:A:LEU:HB2  | 9        | 0.12          |
| (1,739) | 1:4:A:SER:HB3  | 1:59:A:LEU:HB3  | 9        | 0.12          |
| (1,738) | 1:4:A:SER:HB2  | 1:94:A:ALA:H    | 5        | 0.12          |
| (1,738) | 1:4:A:SER:HB2  | 1:94:A:ALA:H    | 16       | 0.12          |
| (1,726) | 1:49:A:LEU:H   | 1:57:A:MET:HG2  | 1        | 0.12          |
| (1,726) | 1:49:A:LEU:H   | 1:57:A:MET:HG2  | 5        | 0.12          |
| (1,726) | 1:49:A:LEU:H   | 1:57:A:MET:HG2  | 9        | 0.12          |
| (1,726) | 1:49:A:LEU:H   | 1:57:A:MET:HG2  | 15       | 0.12          |
| (1,726) | 1:49:A:LEU:H   | 1:57:A:MET:HG2  | 19       | 0.12          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,724) | 1:49:A:LEU:H   | 1:57:A:MET:HA   | 11       | 0.12          |
| (1,724) | 1:49:A:LEU:H   | 1:57:A:MET:HA   | 12       | 0.12          |
| (1,724) | 1:49:A:LEU:H   | 1:57:A:MET:HA   | 18       | 0.12          |
| (1,707) | 1:49:A:LEU:HA  | 1:49:A:LEU:HG   | 20       | 0.12          |
| (1,704) | 1:48:A:LEU:HB2 | 1:48:A:LEU:H    | 3        | 0.12          |
| (1,704) | 1:48:A:LEU:HB3 | 1:48:A:LEU:H    | 3        | 0.12          |
| (1,704) | 1:48:A:LEU:HB2 | 1:48:A:LEU:H    | 6        | 0.12          |
| (1,704) | 1:48:A:LEU:HB3 | 1:48:A:LEU:H    | 6        | 0.12          |
| (1,704) | 1:48:A:LEU:HB2 | 1:48:A:LEU:H    | 11       | 0.12          |
| (1,704) | 1:48:A:LEU:HB3 | 1:48:A:LEU:H    | 11       | 0.12          |
| (1,704) | 1:48:A:LEU:HB2 | 1:48:A:LEU:H    | 12       | 0.12          |
| (1,704) | 1:48:A:LEU:HB3 | 1:48:A:LEU:H    | 12       | 0.12          |
| (1,704) | 1:48:A:LEU:HB2 | 1:48:A:LEU:H    | 14       | 0.12          |
| (1,704) | 1:48:A:LEU:HB3 | 1:48:A:LEU:H    | 14       | 0.12          |
| (1,673) | 1:45:A:ASN:H   | 1:70:A:MET:HB3  | 1        | 0.12          |
| (1,673) | 1:45:A:ASN:H   | 1:70:A:MET:HB3  | 6        | 0.12          |
| (1,601) | 1:3:A:ARG:HG2  | 1:61:A:SER:H    | 2        | 0.12          |
| (1,601) | 1:3:A:ARG:HG2  | 1:61:A:SER:H    | 8        | 0.12          |
| (1,601) | 1:3:A:ARG:HG2  | 1:61:A:SER:H    | 9        | 0.12          |
| (1,601) | 1:3:A:ARG:HG2  | 1:61:A:SER:H    | 18       | 0.12          |
| (1,601) | 1:3:A:ARG:HG2  | 1:61:A:SER:H    | 20       | 0.12          |
| (1,571) | 1:39:A:ILE:H   | 1:46:A:CYS:H    | 6        | 0.12          |
| (1,534) | 1:38:A:PHE:HD1 | 1:45:A:ASN:HB2  | 9        | 0.12          |
| (1,534) | 1:38:A:PHE:HD1 | 1:45:A:ASN:HB3  | 9        | 0.12          |
| (1,534) | 1:38:A:PHE:HD2 | 1:45:A:ASN:HB2  | 9        | 0.12          |
| (1,534) | 1:38:A:PHE:HD2 | 1:45:A:ASN:HB3  | 9        | 0.12          |
| (1,521) | 1:38:A:PHE:HA  | 1:46:A:CYS:H    | 10       | 0.12          |
| (1,493) | 1:36:A:ARG:HA  | 1:49:A:LEU:HA   | 5        | 0.12          |
| (1,472) | 1:34:A:PRO:HB3 | 1:35:A:GLU:H    | 1        | 0.12          |
| (1,472) | 1:34:A:PRO:HB3 | 1:35:A:GLU:H    | 4        | 0.12          |
| (1,472) | 1:34:A:PRO:HB3 | 1:35:A:GLU:H    | 6        | 0.12          |
| (1,472) | 1:34:A:PRO:HB3 | 1:35:A:GLU:H    | 8        | 0.12          |
| (1,472) | 1:34:A:PRO:HB3 | 1:35:A:GLU:H    | 9        | 0.12          |
| (1,472) | 1:34:A:PRO:HB3 | 1:35:A:GLU:H    | 12       | 0.12          |
| (1,472) | 1:34:A:PRO:HB3 | 1:35:A:GLU:H    | 14       | 0.12          |
| (1,472) | 1:34:A:PRO:HB3 | 1:35:A:GLU:H    | 15       | 0.12          |
| (1,472) | 1:34:A:PRO:HB3 | 1:35:A:GLU:H    | 19       | 0.12          |
| (1,437) | 1:32:A:LEU:HB3 | 1:32:A:LEU:H    | 14       | 0.12          |
| (1,398) | 1:30:A:VAL:HA  | 1:30:A:VAL:HG11 | 4        | 0.12          |
| (1,398) | 1:30:A:VAL:HA  | 1:30:A:VAL:HG12 | 4        | 0.12          |
| (1,398) | 1:30:A:VAL:HA  | 1:30:A:VAL:HG13 | 4        | 0.12          |
| (1,372) | 1:29:A:GLU:H   | 1:41:A:PHE:HA   | 17       | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,295) | 1:24:A:TRP:H    | 1:39:A:ILE:HG21 | 9        | 0.12          |
| (1,295) | 1:24:A:TRP:H    | 1:39:A:ILE:HG22 | 9        | 0.12          |
| (1,295) | 1:24:A:TRP:H    | 1:39:A:ILE:HG23 | 9        | 0.12          |
| (1,222) | 1:20:A:LEU:HD11 | 1:24:A:TRP:H    | 20       | 0.12          |
| (1,222) | 1:20:A:LEU:HD12 | 1:24:A:TRP:H    | 20       | 0.12          |
| (1,222) | 1:20:A:LEU:HD13 | 1:24:A:TRP:H    | 20       | 0.12          |
| (1,195) | 1:19:A:ARG:H    | 1:20:A:LEU:H    | 20       | 0.12          |
| (1,194) | 1:19:A:ARG:H    | 1:20:A:LEU:HG   | 1        | 0.12          |
| (1,194) | 1:19:A:ARG:H    | 1:20:A:LEU:HG   | 3        | 0.12          |
| (1,194) | 1:19:A:ARG:H    | 1:20:A:LEU:HG   | 9        | 0.12          |
| (1,176) | 1:18:A:ASN:H    | 1:19:A:ARG:H    | 20       | 0.12          |
| (1,160) | 1:17:A:VAL:HG21 | 1:36:A:ARG:H    | 9        | 0.12          |
| (1,160) | 1:17:A:VAL:HG22 | 1:36:A:ARG:H    | 9        | 0.12          |
| (1,160) | 1:17:A:VAL:HG23 | 1:36:A:ARG:H    | 9        | 0.12          |
| (1,151) | 1:17:A:VAL:HG11 | 1:18:A:ASN:H    | 15       | 0.12          |
| (1,151) | 1:17:A:VAL:HG12 | 1:18:A:ASN:H    | 15       | 0.12          |
| (1,151) | 1:17:A:VAL:HG13 | 1:18:A:ASN:H    | 15       | 0.12          |
| (1,134) | 1:16:A:TYR:H    | 1:17:A:VAL:HB   | 13       | 0.12          |
| (1,120) | 1:16:A:TYR:HA   | 1:16:A:TYR:HD1  | 18       | 0.12          |
| (1,120) | 1:16:A:TYR:HA   | 1:16:A:TYR:HD2  | 18       | 0.12          |
| (1,116) | 1:15:A:ARG:HG2  | 1:16:A:TYR:H    | 11       | 0.12          |
| (1,116) | 1:15:A:ARG:HG3  | 1:16:A:TYR:H    | 11       | 0.12          |
| (1,116) | 1:15:A:ARG:HG2  | 1:16:A:TYR:H    | 12       | 0.12          |
| (1,116) | 1:15:A:ARG:HG3  | 1:16:A:TYR:H    | 12       | 0.12          |
| (1,116) | 1:15:A:ARG:HG2  | 1:16:A:TYR:H    | 15       | 0.12          |
| (1,116) | 1:15:A:ARG:HG3  | 1:16:A:TYR:H    | 15       | 0.12          |
| (1,113) | 1:15:A:ARG:HD2  | 1:20:A:LEU:H    | 15       | 0.12          |
| (1,113) | 1:15:A:ARG:HD3  | 1:20:A:LEU:H    | 15       | 0.12          |
| (1,98)  | 1:15:A:ARG:HB3  | 1:17:A:VAL:H    | 5        | 0.12          |
| (1,98)  | 1:15:A:ARG:HB3  | 1:17:A:VAL:H    | 20       | 0.12          |
| (1,96)  | 1:15:A:ARG:HA   | 1:19:A:ARG:H    | 1        | 0.12          |
| (1,96)  | 1:15:A:ARG:HA   | 1:19:A:ARG:H    | 3        | 0.12          |
| (1,96)  | 1:15:A:ARG:HA   | 1:19:A:ARG:H    | 8        | 0.12          |
| (1,96)  | 1:15:A:ARG:HA   | 1:19:A:ARG:H    | 9        | 0.12          |
| (1,96)  | 1:15:A:ARG:HA   | 1:19:A:ARG:H    | 19       | 0.12          |
| (1,56)  | 1:13:A:ALA:HB1  | 1:16:A:TYR:HD1  | 2        | 0.12          |
| (1,56)  | 1:13:A:ALA:HB1  | 1:16:A:TYR:HD2  | 2        | 0.12          |
| (1,56)  | 1:13:A:ALA:HB2  | 1:16:A:TYR:HD1  | 2        | 0.12          |
| (1,56)  | 1:13:A:ALA:HB2  | 1:16:A:TYR:HD2  | 2        | 0.12          |
| (1,56)  | 1:13:A:ALA:HB3  | 1:16:A:TYR:HD1  | 2        | 0.12          |
| (1,56)  | 1:13:A:ALA:HB3  | 1:16:A:TYR:HD2  | 2        | 0.12          |
| (1,56)  | 1:13:A:ALA:HB1  | 1:16:A:TYR:HD1  | 4        | 0.12          |

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| Key    | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|--------|-----------------|----------------|----------|---------------|
| (1,56) | 1:13:A:ALA:HB1  | 1:16:A:TYR:HD2 | 4        | 0.12          |
| (1,56) | 1:13:A:ALA:HB2  | 1:16:A:TYR:HD1 | 4        | 0.12          |
| (1,56) | 1:13:A:ALA:HB2  | 1:16:A:TYR:HD2 | 4        | 0.12          |
| (1,56) | 1:13:A:ALA:HB3  | 1:16:A:TYR:HD1 | 4        | 0.12          |
| (1,56) | 1:13:A:ALA:HB3  | 1:16:A:TYR:HD2 | 4        | 0.12          |
| (1,56) | 1:13:A:ALA:HB1  | 1:16:A:TYR:HD1 | 12       | 0.12          |
| (1,56) | 1:13:A:ALA:HB1  | 1:16:A:TYR:HD2 | 12       | 0.12          |
| (1,56) | 1:13:A:ALA:HB2  | 1:16:A:TYR:HD1 | 12       | 0.12          |
| (1,56) | 1:13:A:ALA:HB2  | 1:16:A:TYR:HD2 | 12       | 0.12          |
| (1,56) | 1:13:A:ALA:HB3  | 1:16:A:TYR:HD1 | 12       | 0.12          |
| (1,56) | 1:13:A:ALA:HB3  | 1:16:A:TYR:HD2 | 12       | 0.12          |
| (1,56) | 1:13:A:ALA:HB1  | 1:16:A:TYR:HD1 | 13       | 0.12          |
| (1,56) | 1:13:A:ALA:HB1  | 1:16:A:TYR:HD2 | 13       | 0.12          |
| (1,56) | 1:13:A:ALA:HB2  | 1:16:A:TYR:HD1 | 13       | 0.12          |
| (1,56) | 1:13:A:ALA:HB2  | 1:16:A:TYR:HD2 | 13       | 0.12          |
| (1,56) | 1:13:A:ALA:HB3  | 1:16:A:TYR:HD1 | 13       | 0.12          |
| (1,56) | 1:13:A:ALA:HB3  | 1:16:A:TYR:HD2 | 13       | 0.12          |
| (1,5)  | 1:10:A:THR:HG21 | 1:13:A:ALA:HA  | 5        | 0.12          |
| (1,5)  | 1:10:A:THR:HG22 | 1:13:A:ALA:HA  | 5        | 0.12          |
| (1,5)  | 1:10:A:THR:HG23 | 1:13:A:ALA:HA  | 5        | 0.12          |
| (1,5)  | 1:10:A:THR:HG21 | 1:13:A:ALA:HA  | 7        | 0.12          |
| (1,5)  | 1:10:A:THR:HG22 | 1:13:A:ALA:HA  | 7        | 0.12          |
| (1,5)  | 1:10:A:THR:HG23 | 1:13:A:ALA:HA  | 7        | 0.12          |
| (1,5)  | 1:10:A:THR:HG21 | 1:13:A:ALA:HA  | 8        | 0.12          |
| (1,5)  | 1:10:A:THR:HG22 | 1:13:A:ALA:HA  | 8        | 0.12          |
| (1,5)  | 1:10:A:THR:HG23 | 1:13:A:ALA:HA  | 8        | 0.12          |
| (1,5)  | 1:10:A:THR:HG21 | 1:13:A:ALA:HA  | 9        | 0.12          |
| (1,5)  | 1:10:A:THR:HG22 | 1:13:A:ALA:HA  | 9        | 0.12          |
| (1,5)  | 1:10:A:THR:HG23 | 1:13:A:ALA:HA  | 9        | 0.12          |
| (1,5)  | 1:10:A:THR:HG21 | 1:13:A:ALA:HA  | 10       | 0.12          |
| (1,5)  | 1:10:A:THR:HG22 | 1:13:A:ALA:HA  | 10       | 0.12          |
| (1,5)  | 1:10:A:THR:HG23 | 1:13:A:ALA:HA  | 10       | 0.12          |
| (1,5)  | 1:10:A:THR:HG21 | 1:13:A:ALA:HA  | 11       | 0.12          |
| (1,5)  | 1:10:A:THR:HG22 | 1:13:A:ALA:HA  | 11       | 0.12          |
| (1,5)  | 1:10:A:THR:HG23 | 1:13:A:ALA:HA  | 11       | 0.12          |
| (1,5)  | 1:10:A:THR:HG21 | 1:13:A:ALA:HA  | 12       | 0.12          |
| (1,5)  | 1:10:A:THR:HG22 | 1:13:A:ALA:HA  | 12       | 0.12          |
| (1,5)  | 1:10:A:THR:HG23 | 1:13:A:ALA:HA  | 12       | 0.12          |
| (1,5)  | 1:10:A:THR:HG21 | 1:13:A:ALA:HA  | 15       | 0.12          |
| (1,5)  | 1:10:A:THR:HG22 | 1:13:A:ALA:HA  | 15       | 0.12          |
| (1,5)  | 1:10:A:THR:HG23 | 1:13:A:ALA:HA  | 15       | 0.12          |
| (1,5)  | 1:10:A:THR:HG21 | 1:13:A:ALA:HA  | 17       | 0.12          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (1,5)    | 1:10:A:THR:HG22 | 1:13:A:ALA:HA | 17       | 0.12          |
| (1,5)    | 1:10:A:THR:HG23 | 1:13:A:ALA:HA | 17       | 0.12          |
| (1,5)    | 1:10:A:THR:HG21 | 1:13:A:ALA:HA | 19       | 0.12          |
| (1,5)    | 1:10:A:THR:HG22 | 1:13:A:ALA:HA | 19       | 0.12          |
| (1,5)    | 1:10:A:THR:HG23 | 1:13:A:ALA:HA | 19       | 0.12          |
| (1,1386) | 1:9:A:ARG:HA    | 1:54:A:HIS:HA | 9        | 0.11          |
| (1,1342) | 1:90:A:ALA:HB1  | 1:90:A:ALA:H  | 4        | 0.11          |
| (1,1342) | 1:90:A:ALA:HB2  | 1:90:A:ALA:H  | 4        | 0.11          |
| (1,1342) | 1:90:A:ALA:HB3  | 1:90:A:ALA:H  | 4        | 0.11          |
| (1,1342) | 1:90:A:ALA:HB1  | 1:90:A:ALA:H  | 9        | 0.11          |
| (1,1342) | 1:90:A:ALA:HB2  | 1:90:A:ALA:H  | 9        | 0.11          |
| (1,1342) | 1:90:A:ALA:HB3  | 1:90:A:ALA:H  | 9        | 0.11          |
| (1,1342) | 1:90:A:ALA:HB1  | 1:90:A:ALA:H  | 10       | 0.11          |
| (1,1342) | 1:90:A:ALA:HB2  | 1:90:A:ALA:H  | 10       | 0.11          |
| (1,1342) | 1:90:A:ALA:HB3  | 1:90:A:ALA:H  | 10       | 0.11          |
| (1,1342) | 1:90:A:ALA:HB1  | 1:90:A:ALA:H  | 12       | 0.11          |
| (1,1342) | 1:90:A:ALA:HB2  | 1:90:A:ALA:H  | 12       | 0.11          |
| (1,1342) | 1:90:A:ALA:HB3  | 1:90:A:ALA:H  | 12       | 0.11          |
| (1,1342) | 1:90:A:ALA:HB1  | 1:90:A:ALA:H  | 14       | 0.11          |
| (1,1342) | 1:90:A:ALA:HB2  | 1:90:A:ALA:H  | 14       | 0.11          |
| (1,1342) | 1:90:A:ALA:HB3  | 1:90:A:ALA:H  | 14       | 0.11          |
| (1,1315) | 1:87:A:LEU:HG   | 1:87:A:LEU:H  | 8        | 0.11          |
| (1,1315) | 1:87:A:LEU:HG   | 1:87:A:LEU:H  | 20       | 0.11          |
| (1,1309) | 1:87:A:LEU:HB2  | 1:87:A:LEU:H  | 8        | 0.11          |
| (1,1309) | 1:87:A:LEU:HB2  | 1:87:A:LEU:H  | 12       | 0.11          |
| (1,1309) | 1:87:A:LEU:HB2  | 1:87:A:LEU:H  | 13       | 0.11          |
| (1,1309) | 1:87:A:LEU:HB2  | 1:87:A:LEU:H  | 20       | 0.11          |
| (1,1308) | 1:87:A:LEU:HB3  | 1:89:A:ILE:HA | 1        | 0.11          |
| (1,1308) | 1:87:A:LEU:HB3  | 1:89:A:ILE:HA | 2        | 0.11          |
| (1,1308) | 1:87:A:LEU:HB3  | 1:89:A:ILE:HA | 3        | 0.11          |
| (1,1308) | 1:87:A:LEU:HB3  | 1:89:A:ILE:HA | 7        | 0.11          |
| (1,1308) | 1:87:A:LEU:HB3  | 1:89:A:ILE:HA | 8        | 0.11          |
| (1,1308) | 1:87:A:LEU:HB3  | 1:89:A:ILE:HA | 9        | 0.11          |
| (1,1308) | 1:87:A:LEU:HB3  | 1:89:A:ILE:HA | 11       | 0.11          |
| (1,1308) | 1:87:A:LEU:HB3  | 1:89:A:ILE:HA | 12       | 0.11          |
| (1,1308) | 1:87:A:LEU:HB3  | 1:89:A:ILE:HA | 18       | 0.11          |
| (1,1283) | 1:81:A:MET:HB3  | 1:82:A:ALA:H  | 6        | 0.11          |
| (1,1276) | 1:80:A:ARG:HG2  | 1:81:A:MET:H  | 1        | 0.11          |
| (1,1145) | 1:74:A:VAL:HB   | 1:76:A:ASP:H  | 4        | 0.11          |
| (1,1145) | 1:74:A:VAL:HB   | 1:76:A:ASP:H  | 5        | 0.11          |
| (1,1145) | 1:74:A:VAL:HB   | 1:76:A:ASP:H  | 7        | 0.11          |
| (1,1145) | 1:74:A:VAL:HB   | 1:76:A:ASP:H  | 11       | 0.11          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1145) | 1:74:A:VAL:HB  | 1:76:A:ASP:H    | 12       | 0.11          |
| (1,1145) | 1:74:A:VAL:HB  | 1:76:A:ASP:H    | 20       | 0.11          |
| (1,1063) | 1:6:A:SER:H    | 1:58:A:ILE:HG21 | 2        | 0.11          |
| (1,1063) | 1:6:A:SER:H    | 1:58:A:ILE:HG22 | 2        | 0.11          |
| (1,1063) | 1:6:A:SER:H    | 1:58:A:ILE:HG23 | 2        | 0.11          |
| (1,1063) | 1:6:A:SER:H    | 1:58:A:ILE:HG21 | 3        | 0.11          |
| (1,1063) | 1:6:A:SER:H    | 1:58:A:ILE:HG22 | 3        | 0.11          |
| (1,1063) | 1:6:A:SER:H    | 1:58:A:ILE:HG23 | 3        | 0.11          |
| (1,1063) | 1:6:A:SER:H    | 1:58:A:ILE:HG21 | 6        | 0.11          |
| (1,1063) | 1:6:A:SER:H    | 1:58:A:ILE:HG22 | 6        | 0.11          |
| (1,1063) | 1:6:A:SER:H    | 1:58:A:ILE:HG23 | 6        | 0.11          |
| (1,1063) | 1:6:A:SER:H    | 1:58:A:ILE:HG21 | 7        | 0.11          |
| (1,1063) | 1:6:A:SER:H    | 1:58:A:ILE:HG22 | 7        | 0.11          |
| (1,1063) | 1:6:A:SER:H    | 1:58:A:ILE:HG23 | 7        | 0.11          |
| (1,1063) | 1:6:A:SER:H    | 1:58:A:ILE:HG21 | 14       | 0.11          |
| (1,1063) | 1:6:A:SER:H    | 1:58:A:ILE:HG22 | 14       | 0.11          |
| (1,1063) | 1:6:A:SER:H    | 1:58:A:ILE:HG23 | 14       | 0.11          |
| (1,1063) | 1:6:A:SER:H    | 1:58:A:ILE:HG21 | 18       | 0.11          |
| (1,1063) | 1:6:A:SER:H    | 1:58:A:ILE:HG22 | 18       | 0.11          |
| (1,1063) | 1:6:A:SER:H    | 1:58:A:ILE:HG23 | 18       | 0.11          |
| (1,1063) | 1:6:A:SER:H    | 1:58:A:ILE:HG21 | 20       | 0.11          |
| (1,1063) | 1:6:A:SER:H    | 1:58:A:ILE:HG22 | 20       | 0.11          |
| (1,1063) | 1:6:A:SER:H    | 1:58:A:ILE:HG23 | 20       | 0.11          |
| (1,992)  | 1:66:A:SER:H   | 1:67:A:LEU:H    | 7        | 0.11          |
| (1,992)  | 1:66:A:SER:H   | 1:67:A:LEU:H    | 12       | 0.11          |
| (1,992)  | 1:66:A:SER:H   | 1:67:A:LEU:H    | 19       | 0.11          |
| (1,964)  | 1:64:A:GLU:HG2 | 1:67:A:LEU:HG   | 1        | 0.11          |
| (1,964)  | 1:64:A:GLU:HG3 | 1:67:A:LEU:HG   | 1        | 0.11          |
| (1,964)  | 1:64:A:GLU:HG2 | 1:67:A:LEU:HG   | 8        | 0.11          |
| (1,964)  | 1:64:A:GLU:HG3 | 1:67:A:LEU:HG   | 8        | 0.11          |
| (1,964)  | 1:64:A:GLU:HG2 | 1:67:A:LEU:HG   | 20       | 0.11          |
| (1,964)  | 1:64:A:GLU:HG3 | 1:67:A:LEU:HG   | 20       | 0.11          |
| (1,954)  | 1:64:A:GLU:HA  | 1:67:A:LEU:HG   | 1        | 0.11          |
| (1,954)  | 1:64:A:GLU:HA  | 1:67:A:LEU:HG   | 2        | 0.11          |
| (1,954)  | 1:64:A:GLU:HA  | 1:67:A:LEU:HG   | 6        | 0.11          |
| (1,954)  | 1:64:A:GLU:HA  | 1:67:A:LEU:HG   | 8        | 0.11          |
| (1,954)  | 1:64:A:GLU:HA  | 1:67:A:LEU:HG   | 9        | 0.11          |
| (1,954)  | 1:64:A:GLU:HA  | 1:67:A:LEU:HG   | 10       | 0.11          |
| (1,954)  | 1:64:A:GLU:HA  | 1:67:A:LEU:HG   | 15       | 0.11          |
| (1,954)  | 1:64:A:GLU:HA  | 1:67:A:LEU:HG   | 18       | 0.11          |
| (1,954)  | 1:64:A:GLU:HA  | 1:67:A:LEU:HG   | 20       | 0.11          |
| (1,938)  | 1:63:A:ASP:H   | 1:66:A:SER:HA   | 5        | 0.11          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,938) | 1:63:A:ASP:H   | 1:66:A:SER:HA  | 13       | 0.11          |
| (1,938) | 1:63:A:ASP:H   | 1:66:A:SER:HA  | 14       | 0.11          |
| (1,938) | 1:63:A:ASP:H   | 1:66:A:SER:HA  | 16       | 0.11          |
| (1,938) | 1:63:A:ASP:H   | 1:66:A:SER:HA  | 18       | 0.11          |
| (1,938) | 1:63:A:ASP:H   | 1:66:A:SER:HA  | 19       | 0.11          |
| (1,938) | 1:63:A:ASP:H   | 1:66:A:SER:HA  | 20       | 0.11          |
| (1,914) | 1:61:A:SER:HB2 | 1:67:A:LEU:HA  | 15       | 0.11          |
| (1,914) | 1:61:A:SER:HB3 | 1:67:A:LEU:HA  | 15       | 0.11          |
| (1,832) | 1:57:A:MET:HA  | 1:58:A:ILE:H   | 20       | 0.11          |
| (1,800) | 1:54:A:HIS:HA  | 1:55:A:VAL:H   | 13       | 0.11          |
| (1,791) | 1:52:A:PRO:HD2 | 1:54:A:HIS:H   | 16       | 0.11          |
| (1,774) | 1:51:A:HIS:H   | 1:52:A:PRO:HD2 | 1        | 0.11          |
| (1,774) | 1:51:A:HIS:H   | 1:52:A:PRO:HD2 | 2        | 0.11          |
| (1,774) | 1:51:A:HIS:H   | 1:52:A:PRO:HD2 | 3        | 0.11          |
| (1,774) | 1:51:A:HIS:H   | 1:52:A:PRO:HD2 | 4        | 0.11          |
| (1,774) | 1:51:A:HIS:H   | 1:52:A:PRO:HD2 | 5        | 0.11          |
| (1,774) | 1:51:A:HIS:H   | 1:52:A:PRO:HD2 | 6        | 0.11          |
| (1,774) | 1:51:A:HIS:H   | 1:52:A:PRO:HD2 | 7        | 0.11          |
| (1,774) | 1:51:A:HIS:H   | 1:52:A:PRO:HD2 | 8        | 0.11          |
| (1,774) | 1:51:A:HIS:H   | 1:52:A:PRO:HD2 | 14       | 0.11          |
| (1,774) | 1:51:A:HIS:H   | 1:52:A:PRO:HD2 | 15       | 0.11          |
| (1,774) | 1:51:A:HIS:H   | 1:52:A:PRO:HD2 | 17       | 0.11          |
| (1,774) | 1:51:A:HIS:H   | 1:52:A:PRO:HD2 | 18       | 0.11          |
| (1,774) | 1:51:A:HIS:H   | 1:52:A:PRO:HD2 | 19       | 0.11          |
| (1,774) | 1:51:A:HIS:H   | 1:52:A:PRO:HD2 | 20       | 0.11          |
| (1,773) | 1:51:A:HIS:H   | 1:52:A:PRO:HD3 | 1        | 0.11          |
| (1,773) | 1:51:A:HIS:H   | 1:52:A:PRO:HD3 | 2        | 0.11          |
| (1,773) | 1:51:A:HIS:H   | 1:52:A:PRO:HD3 | 3        | 0.11          |
| (1,773) | 1:51:A:HIS:H   | 1:52:A:PRO:HD3 | 4        | 0.11          |
| (1,773) | 1:51:A:HIS:H   | 1:52:A:PRO:HD3 | 5        | 0.11          |
| (1,773) | 1:51:A:HIS:H   | 1:52:A:PRO:HD3 | 8        | 0.11          |
| (1,773) | 1:51:A:HIS:H   | 1:52:A:PRO:HD3 | 9        | 0.11          |
| (1,773) | 1:51:A:HIS:H   | 1:52:A:PRO:HD3 | 10       | 0.11          |
| (1,773) | 1:51:A:HIS:H   | 1:52:A:PRO:HD3 | 16       | 0.11          |
| (1,773) | 1:51:A:HIS:H   | 1:52:A:PRO:HD3 | 17       | 0.11          |
| (1,773) | 1:51:A:HIS:H   | 1:52:A:PRO:HD3 | 19       | 0.11          |
| (1,773) | 1:51:A:HIS:H   | 1:52:A:PRO:HD3 | 20       | 0.11          |
| (1,739) | 1:4:A:SER:HB2  | 1:59:A:LEU:HB2 | 1        | 0.11          |
| (1,739) | 1:4:A:SER:HB2  | 1:59:A:LEU:HB3 | 1        | 0.11          |
| (1,739) | 1:4:A:SER:HB3  | 1:59:A:LEU:HB2 | 1        | 0.11          |
| (1,739) | 1:4:A:SER:HB3  | 1:59:A:LEU:HB3 | 1        | 0.11          |
| (1,739) | 1:4:A:SER:HB2  | 1:59:A:LEU:HB2 | 3        | 0.11          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,739) | 1:4:A:SER:HB2 | 1:59:A:LEU:HB3 | 3        | 0.11          |
| (1,739) | 1:4:A:SER:HB3 | 1:59:A:LEU:HB2 | 3        | 0.11          |
| (1,739) | 1:4:A:SER:HB3 | 1:59:A:LEU:HB3 | 3        | 0.11          |
| (1,739) | 1:4:A:SER:HB2 | 1:59:A:LEU:HB2 | 4        | 0.11          |
| (1,739) | 1:4:A:SER:HB2 | 1:59:A:LEU:HB3 | 4        | 0.11          |
| (1,739) | 1:4:A:SER:HB3 | 1:59:A:LEU:HB2 | 4        | 0.11          |
| (1,739) | 1:4:A:SER:HB3 | 1:59:A:LEU:HB3 | 4        | 0.11          |
| (1,739) | 1:4:A:SER:HB2 | 1:59:A:LEU:HB2 | 7        | 0.11          |
| (1,739) | 1:4:A:SER:HB2 | 1:59:A:LEU:HB3 | 7        | 0.11          |
| (1,739) | 1:4:A:SER:HB3 | 1:59:A:LEU:HB2 | 7        | 0.11          |
| (1,739) | 1:4:A:SER:HB3 | 1:59:A:LEU:HB3 | 7        | 0.11          |
| (1,739) | 1:4:A:SER:HB2 | 1:59:A:LEU:HB2 | 11       | 0.11          |
| (1,739) | 1:4:A:SER:HB2 | 1:59:A:LEU:HB3 | 11       | 0.11          |
| (1,739) | 1:4:A:SER:HB3 | 1:59:A:LEU:HB2 | 11       | 0.11          |
| (1,739) | 1:4:A:SER:HB3 | 1:59:A:LEU:HB3 | 11       | 0.11          |
| (1,739) | 1:4:A:SER:HB2 | 1:59:A:LEU:HB2 | 12       | 0.11          |
| (1,739) | 1:4:A:SER:HB2 | 1:59:A:LEU:HB3 | 12       | 0.11          |
| (1,739) | 1:4:A:SER:HB3 | 1:59:A:LEU:HB2 | 12       | 0.11          |
| (1,739) | 1:4:A:SER:HB3 | 1:59:A:LEU:HB3 | 12       | 0.11          |
| (1,739) | 1:4:A:SER:HB2 | 1:59:A:LEU:HB2 | 13       | 0.11          |
| (1,739) | 1:4:A:SER:HB2 | 1:59:A:LEU:HB3 | 13       | 0.11          |
| (1,739) | 1:4:A:SER:HB3 | 1:59:A:LEU:HB2 | 13       | 0.11          |
| (1,739) | 1:4:A:SER:HB3 | 1:59:A:LEU:HB3 | 13       | 0.11          |
| (1,739) | 1:4:A:SER:HB2 | 1:59:A:LEU:HB2 | 17       | 0.11          |
| (1,739) | 1:4:A:SER:HB2 | 1:59:A:LEU:HB3 | 17       | 0.11          |
| (1,739) | 1:4:A:SER:HB3 | 1:59:A:LEU:HB2 | 17       | 0.11          |
| (1,739) | 1:4:A:SER:HB3 | 1:59:A:LEU:HB3 | 17       | 0.11          |
| (1,739) | 1:4:A:SER:HB2 | 1:59:A:LEU:HB2 | 18       | 0.11          |
| (1,739) | 1:4:A:SER:HB2 | 1:59:A:LEU:HB3 | 18       | 0.11          |
| (1,739) | 1:4:A:SER:HB3 | 1:59:A:LEU:HB2 | 18       | 0.11          |
| (1,739) | 1:4:A:SER:HB3 | 1:59:A:LEU:HB3 | 18       | 0.11          |
| (1,739) | 1:4:A:SER:HB2 | 1:59:A:LEU:HB2 | 20       | 0.11          |
| (1,739) | 1:4:A:SER:HB2 | 1:59:A:LEU:HB3 | 20       | 0.11          |
| (1,739) | 1:4:A:SER:HB3 | 1:59:A:LEU:HB2 | 20       | 0.11          |
| (1,739) | 1:4:A:SER:HB3 | 1:59:A:LEU:HB3 | 20       | 0.11          |
| (1,738) | 1:4:A:SER:HB2 | 1:94:A:ALA:H   | 6        | 0.11          |
| (1,738) | 1:4:A:SER:HB2 | 1:94:A:ALA:H   | 11       | 0.11          |
| (1,738) | 1:4:A:SER:HB2 | 1:94:A:ALA:H   | 15       | 0.11          |
| (1,738) | 1:4:A:SER:HB2 | 1:94:A:ALA:H   | 19       | 0.11          |
| (1,726) | 1:49:A:LEU:H  | 1:57:A:MET:HG2 | 20       | 0.11          |
| (1,724) | 1:49:A:LEU:H  | 1:57:A:MET:HA  | 3        | 0.11          |
| (1,724) | 1:49:A:LEU:H  | 1:57:A:MET:HA  | 4        | 0.11          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,724) | 1:49:A:LEU:H   | 1:57:A:MET:HA  | 8        | 0.11          |
| (1,724) | 1:49:A:LEU:H   | 1:57:A:MET:HA  | 14       | 0.11          |
| (1,724) | 1:49:A:LEU:H   | 1:57:A:MET:HA  | 15       | 0.11          |
| (1,692) | 1:47:A:GLU:HG2 | 1:48:A:LEU:H   | 20       | 0.11          |
| (1,692) | 1:47:A:GLU:HG3 | 1:48:A:LEU:H   | 20       | 0.11          |
| (1,673) | 1:45:A:ASN:H   | 1:70:A:MET:HB3 | 16       | 0.11          |
| (1,673) | 1:45:A:ASN:H   | 1:70:A:MET:HB3 | 20       | 0.11          |
| (1,637) | 1:41:A:PHE:H   | 1:46:A:CYS:H   | 10       | 0.11          |
| (1,614) | 1:40:A:ASP:HB3 | 1:40:A:ASP:H   | 2        | 0.11          |
| (1,614) | 1:40:A:ASP:HB3 | 1:40:A:ASP:H   | 15       | 0.11          |
| (1,601) | 1:3:A:ARG:HG2  | 1:61:A:SER:H   | 1        | 0.11          |
| (1,601) | 1:3:A:ARG:HG2  | 1:61:A:SER:H   | 3        | 0.11          |
| (1,601) | 1:3:A:ARG:HG2  | 1:61:A:SER:H   | 6        | 0.11          |
| (1,601) | 1:3:A:ARG:HG2  | 1:61:A:SER:H   | 7        | 0.11          |
| (1,601) | 1:3:A:ARG:HG2  | 1:61:A:SER:H   | 10       | 0.11          |
| (1,601) | 1:3:A:ARG:HG2  | 1:61:A:SER:H   | 11       | 0.11          |
| (1,601) | 1:3:A:ARG:HG2  | 1:61:A:SER:H   | 12       | 0.11          |
| (1,601) | 1:3:A:ARG:HG2  | 1:61:A:SER:H   | 14       | 0.11          |
| (1,601) | 1:3:A:ARG:HG2  | 1:61:A:SER:H   | 15       | 0.11          |
| (1,601) | 1:3:A:ARG:HG2  | 1:61:A:SER:H   | 17       | 0.11          |
| (1,601) | 1:3:A:ARG:HG2  | 1:61:A:SER:H   | 19       | 0.11          |
| (1,571) | 1:39:A:ILE:H   | 1:46:A:CYS:H   | 11       | 0.11          |
| (1,571) | 1:39:A:ILE:H   | 1:46:A:CYS:H   | 12       | 0.11          |
| (1,534) | 1:38:A:PHE:HD1 | 1:45:A:ASN:HB2 | 5        | 0.11          |
| (1,534) | 1:38:A:PHE:HD1 | 1:45:A:ASN:HB3 | 5        | 0.11          |
| (1,534) | 1:38:A:PHE:HD2 | 1:45:A:ASN:HB2 | 5        | 0.11          |
| (1,534) | 1:38:A:PHE:HD2 | 1:45:A:ASN:HB3 | 5        | 0.11          |
| (1,521) | 1:38:A:PHE:HA  | 1:46:A:CYS:H   | 1        | 0.11          |
| (1,521) | 1:38:A:PHE:HA  | 1:46:A:CYS:H   | 7        | 0.11          |
| (1,521) | 1:38:A:PHE:HA  | 1:46:A:CYS:H   | 9        | 0.11          |
| (1,521) | 1:38:A:PHE:HA  | 1:46:A:CYS:H   | 17       | 0.11          |
| (1,521) | 1:38:A:PHE:HA  | 1:46:A:CYS:H   | 18       | 0.11          |
| (1,511) | 1:37:A:GLY:HA2 | 1:38:A:PHE:H   | 18       | 0.11          |
| (1,493) | 1:36:A:ARG:HA  | 1:49:A:LEU:HA  | 1        | 0.11          |
| (1,493) | 1:36:A:ARG:HA  | 1:49:A:LEU:HA  | 15       | 0.11          |
| (1,493) | 1:36:A:ARG:HA  | 1:49:A:LEU:HA  | 18       | 0.11          |
| (1,493) | 1:36:A:ARG:HA  | 1:49:A:LEU:HA  | 19       | 0.11          |
| (1,472) | 1:34:A:PRO:HB3 | 1:35:A:GLU:H   | 3        | 0.11          |
| (1,472) | 1:34:A:PRO:HB3 | 1:35:A:GLU:H   | 5        | 0.11          |
| (1,472) | 1:34:A:PRO:HB3 | 1:35:A:GLU:H   | 11       | 0.11          |
| (1,472) | 1:34:A:PRO:HB3 | 1:35:A:GLU:H   | 17       | 0.11          |
| (1,472) | 1:34:A:PRO:HB3 | 1:35:A:GLU:H   | 20       | 0.11          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,470) | 1:34:A:PRO:HA  | 1:34:A:PRO:HG2  | 18       | 0.11          |
| (1,437) | 1:32:A:LEU:HB3 | 1:32:A:LEU:H    | 12       | 0.11          |
| (1,398) | 1:30:A:VAL:HA  | 1:30:A:VAL:HG11 | 6        | 0.11          |
| (1,398) | 1:30:A:VAL:HA  | 1:30:A:VAL:HG12 | 6        | 0.11          |
| (1,398) | 1:30:A:VAL:HA  | 1:30:A:VAL:HG13 | 6        | 0.11          |
| (1,398) | 1:30:A:VAL:HA  | 1:30:A:VAL:HG11 | 8        | 0.11          |
| (1,398) | 1:30:A:VAL:HA  | 1:30:A:VAL:HG12 | 8        | 0.11          |
| (1,398) | 1:30:A:VAL:HA  | 1:30:A:VAL:HG13 | 8        | 0.11          |
| (1,394) | 1:2:A:PHE:H    | 1:62:A:PRO:HD2  | 12       | 0.11          |
| (1,394) | 1:2:A:PHE:H    | 1:62:A:PRO:HD3  | 12       | 0.11          |
| (1,374) | 1:2:A:PHE:HB3  | 1:3:A:ARG:H     | 9        | 0.11          |
| (1,335) | 1:28:A:PHE:HA  | 1:30:A:VAL:HG21 | 20       | 0.11          |
| (1,335) | 1:28:A:PHE:HA  | 1:30:A:VAL:HG22 | 20       | 0.11          |
| (1,335) | 1:28:A:PHE:HA  | 1:30:A:VAL:HG23 | 20       | 0.11          |
| (1,295) | 1:24:A:TRP:H   | 1:39:A:ILE:HG21 | 6        | 0.11          |
| (1,295) | 1:24:A:TRP:H   | 1:39:A:ILE:HG22 | 6        | 0.11          |
| (1,295) | 1:24:A:TRP:H   | 1:39:A:ILE:HG23 | 6        | 0.11          |
| (1,295) | 1:24:A:TRP:H   | 1:39:A:ILE:HG21 | 8        | 0.11          |
| (1,295) | 1:24:A:TRP:H   | 1:39:A:ILE:HG22 | 8        | 0.11          |
| (1,295) | 1:24:A:TRP:H   | 1:39:A:ILE:HG23 | 8        | 0.11          |
| (1,295) | 1:24:A:TRP:H   | 1:39:A:ILE:HG21 | 11       | 0.11          |
| (1,295) | 1:24:A:TRP:H   | 1:39:A:ILE:HG22 | 11       | 0.11          |
| (1,295) | 1:24:A:TRP:H   | 1:39:A:ILE:HG23 | 11       | 0.11          |
| (1,295) | 1:24:A:TRP:H   | 1:39:A:ILE:HG21 | 12       | 0.11          |
| (1,295) | 1:24:A:TRP:H   | 1:39:A:ILE:HG22 | 12       | 0.11          |
| (1,295) | 1:24:A:TRP:H   | 1:39:A:ILE:HG23 | 12       | 0.11          |
| (1,295) | 1:24:A:TRP:H   | 1:39:A:ILE:HG21 | 13       | 0.11          |
| (1,295) | 1:24:A:TRP:H   | 1:39:A:ILE:HG22 | 13       | 0.11          |
| (1,295) | 1:24:A:TRP:H   | 1:39:A:ILE:HG23 | 13       | 0.11          |
| (1,295) | 1:24:A:TRP:H   | 1:39:A:ILE:HG21 | 14       | 0.11          |
| (1,295) | 1:24:A:TRP:H   | 1:39:A:ILE:HG22 | 14       | 0.11          |
| (1,295) | 1:24:A:TRP:H   | 1:39:A:ILE:HG23 | 14       | 0.11          |
| (1,295) | 1:24:A:TRP:H   | 1:39:A:ILE:HG21 | 16       | 0.11          |
| (1,295) | 1:24:A:TRP:H   | 1:39:A:ILE:HG22 | 16       | 0.11          |
| (1,295) | 1:24:A:TRP:H   | 1:39:A:ILE:HG23 | 16       | 0.11          |
| (1,295) | 1:24:A:TRP:H   | 1:39:A:ILE:HG21 | 17       | 0.11          |
| (1,295) | 1:24:A:TRP:H   | 1:39:A:ILE:HG22 | 17       | 0.11          |
| (1,295) | 1:24:A:TRP:H   | 1:39:A:ILE:HG23 | 17       | 0.11          |
| (1,292) | 1:24:A:TRP:HB2 | 1:39:A:ILE:HG21 | 14       | 0.11          |
| (1,292) | 1:24:A:TRP:HB2 | 1:39:A:ILE:HG22 | 14       | 0.11          |
| (1,292) | 1:24:A:TRP:HB2 | 1:39:A:ILE:HG23 | 14       | 0.11          |
| (1,292) | 1:24:A:TRP:HB3 | 1:39:A:ILE:HG21 | 14       | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,292) | 1:24:A:TRP:HB3  | 1:39:A:ILE:HG22 | 14       | 0.11          |
| (1,292) | 1:24:A:TRP:HB3  | 1:39:A:ILE:HG23 | 14       | 0.11          |
| (1,292) | 1:24:A:TRP:HB2  | 1:39:A:ILE:HG21 | 17       | 0.11          |
| (1,292) | 1:24:A:TRP:HB2  | 1:39:A:ILE:HG22 | 17       | 0.11          |
| (1,292) | 1:24:A:TRP:HB2  | 1:39:A:ILE:HG23 | 17       | 0.11          |
| (1,292) | 1:24:A:TRP:HB3  | 1:39:A:ILE:HG21 | 17       | 0.11          |
| (1,292) | 1:24:A:TRP:HB3  | 1:39:A:ILE:HG22 | 17       | 0.11          |
| (1,292) | 1:24:A:TRP:HB3  | 1:39:A:ILE:HG23 | 17       | 0.11          |
| (1,284) | 1:24:A:TRP:HA   | 1:25:A:GLY:H    | 3        | 0.11          |
| (1,283) | 1:23:A:HIS:H    | 1:30:A:VAL:HG21 | 2        | 0.11          |
| (1,283) | 1:23:A:HIS:H    | 1:30:A:VAL:HG22 | 2        | 0.11          |
| (1,283) | 1:23:A:HIS:H    | 1:30:A:VAL:HG23 | 2        | 0.11          |
| (1,283) | 1:23:A:HIS:H    | 1:30:A:VAL:HG21 | 14       | 0.11          |
| (1,283) | 1:23:A:HIS:H    | 1:30:A:VAL:HG22 | 14       | 0.11          |
| (1,283) | 1:23:A:HIS:H    | 1:30:A:VAL:HG23 | 14       | 0.11          |
| (1,283) | 1:23:A:HIS:H    | 1:30:A:VAL:HG21 | 20       | 0.11          |
| (1,283) | 1:23:A:HIS:H    | 1:30:A:VAL:HG22 | 20       | 0.11          |
| (1,283) | 1:23:A:HIS:H    | 1:30:A:VAL:HG23 | 20       | 0.11          |
| (1,199) | 1:1:A:MET:HA    | 1:62:A:PRO:HA   | 16       | 0.11          |
| (1,195) | 1:19:A:ARG:H    | 1:20:A:LEU:H    | 5        | 0.11          |
| (1,195) | 1:19:A:ARG:H    | 1:20:A:LEU:H    | 18       | 0.11          |
| (1,176) | 1:18:A:ASN:H    | 1:19:A:ARG:H    | 1        | 0.11          |
| (1,176) | 1:18:A:ASN:H    | 1:19:A:ARG:H    | 4        | 0.11          |
| (1,176) | 1:18:A:ASN:H    | 1:19:A:ARG:H    | 6        | 0.11          |
| (1,176) | 1:18:A:ASN:H    | 1:19:A:ARG:H    | 9        | 0.11          |
| (1,176) | 1:18:A:ASN:H    | 1:19:A:ARG:H    | 19       | 0.11          |
| (1,160) | 1:17:A:VAL:HG21 | 1:36:A:ARG:H    | 1        | 0.11          |
| (1,160) | 1:17:A:VAL:HG22 | 1:36:A:ARG:H    | 1        | 0.11          |
| (1,160) | 1:17:A:VAL:HG23 | 1:36:A:ARG:H    | 1        | 0.11          |
| (1,151) | 1:17:A:VAL:HG11 | 1:18:A:ASN:H    | 4        | 0.11          |
| (1,151) | 1:17:A:VAL:HG12 | 1:18:A:ASN:H    | 4        | 0.11          |
| (1,151) | 1:17:A:VAL:HG13 | 1:18:A:ASN:H    | 4        | 0.11          |
| (1,151) | 1:17:A:VAL:HG11 | 1:18:A:ASN:H    | 6        | 0.11          |
| (1,151) | 1:17:A:VAL:HG12 | 1:18:A:ASN:H    | 6        | 0.11          |
| (1,151) | 1:17:A:VAL:HG13 | 1:18:A:ASN:H    | 6        | 0.11          |
| (1,151) | 1:17:A:VAL:HG11 | 1:18:A:ASN:H    | 18       | 0.11          |
| (1,151) | 1:17:A:VAL:HG12 | 1:18:A:ASN:H    | 18       | 0.11          |
| (1,151) | 1:17:A:VAL:HG13 | 1:18:A:ASN:H    | 18       | 0.11          |
| (1,134) | 1:16:A:TYR:H    | 1:17:A:VAL:HB   | 2        | 0.11          |
| (1,120) | 1:16:A:TYR:HA   | 1:16:A:TYR:HD1  | 20       | 0.11          |
| (1,120) | 1:16:A:TYR:HA   | 1:16:A:TYR:HD2  | 20       | 0.11          |
| (1,116) | 1:15:A:ARG:HG2  | 1:16:A:TYR:H    | 4        | 0.11          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,116) | 1:15:A:ARG:HG3 | 1:16:A:TYR:H   | 4        | 0.11          |
| (1,113) | 1:15:A:ARG:HD2 | 1:20:A:LEU:H   | 4        | 0.11          |
| (1,113) | 1:15:A:ARG:HD3 | 1:20:A:LEU:H   | 4        | 0.11          |
| (1,113) | 1:15:A:ARG:HD2 | 1:20:A:LEU:H   | 8        | 0.11          |
| (1,113) | 1:15:A:ARG:HD3 | 1:20:A:LEU:H   | 8        | 0.11          |
| (1,113) | 1:15:A:ARG:HD2 | 1:20:A:LEU:H   | 19       | 0.11          |
| (1,113) | 1:15:A:ARG:HD3 | 1:20:A:LEU:H   | 19       | 0.11          |
| (1,103) | 1:15:A:ARG:HD2 | 1:15:A:ARG:H   | 20       | 0.11          |
| (1,103) | 1:15:A:ARG:HD3 | 1:15:A:ARG:H   | 20       | 0.11          |
| (1,98)  | 1:15:A:ARG:HB3 | 1:17:A:VAL:H   | 18       | 0.11          |
| (1,97)  | 1:15:A:ARG:HB3 | 1:16:A:TYR:H   | 5        | 0.11          |
| (1,97)  | 1:15:A:ARG:HB3 | 1:16:A:TYR:H   | 20       | 0.11          |
| (1,96)  | 1:15:A:ARG:HA  | 1:19:A:ARG:H   | 12       | 0.11          |
| (1,96)  | 1:15:A:ARG:HA  | 1:19:A:ARG:H   | 14       | 0.11          |
| (1,96)  | 1:15:A:ARG:HA  | 1:19:A:ARG:H   | 15       | 0.11          |
| (1,85)  | 1:14:A:ALA:HB1 | 1:50:A:ALA:HA  | 9        | 0.11          |
| (1,85)  | 1:14:A:ALA:HB2 | 1:50:A:ALA:HA  | 9        | 0.11          |
| (1,85)  | 1:14:A:ALA:HB3 | 1:50:A:ALA:HA  | 9        | 0.11          |
| (1,85)  | 1:14:A:ALA:HB1 | 1:50:A:ALA:HA  | 16       | 0.11          |
| (1,85)  | 1:14:A:ALA:HB2 | 1:50:A:ALA:HA  | 16       | 0.11          |
| (1,85)  | 1:14:A:ALA:HB3 | 1:50:A:ALA:HA  | 16       | 0.11          |
| (1,56)  | 1:13:A:ALA:HB1 | 1:16:A:TYR:HD1 | 6        | 0.11          |
| (1,56)  | 1:13:A:ALA:HB1 | 1:16:A:TYR:HD2 | 6        | 0.11          |
| (1,56)  | 1:13:A:ALA:HB2 | 1:16:A:TYR:HD1 | 6        | 0.11          |
| (1,56)  | 1:13:A:ALA:HB2 | 1:16:A:TYR:HD2 | 6        | 0.11          |
| (1,56)  | 1:13:A:ALA:HB3 | 1:16:A:TYR:HD1 | 6        | 0.11          |
| (1,56)  | 1:13:A:ALA:HB3 | 1:16:A:TYR:HD2 | 6        | 0.11          |
| (1,56)  | 1:13:A:ALA:HB1 | 1:16:A:TYR:HD1 | 9        | 0.11          |
| (1,56)  | 1:13:A:ALA:HB1 | 1:16:A:TYR:HD2 | 9        | 0.11          |
| (1,56)  | 1:13:A:ALA:HB2 | 1:16:A:TYR:HD1 | 9        | 0.11          |
| (1,56)  | 1:13:A:ALA:HB2 | 1:16:A:TYR:HD2 | 9        | 0.11          |
| (1,56)  | 1:13:A:ALA:HB3 | 1:16:A:TYR:HD1 | 9        | 0.11          |
| (1,56)  | 1:13:A:ALA:HB3 | 1:16:A:TYR:HD2 | 9        | 0.11          |
| (1,56)  | 1:13:A:ALA:HB1 | 1:16:A:TYR:HD1 | 15       | 0.11          |
| (1,56)  | 1:13:A:ALA:HB1 | 1:16:A:TYR:HD2 | 15       | 0.11          |
| (1,56)  | 1:13:A:ALA:HB2 | 1:16:A:TYR:HD1 | 15       | 0.11          |
| (1,56)  | 1:13:A:ALA:HB2 | 1:16:A:TYR:HD2 | 15       | 0.11          |
| (1,56)  | 1:13:A:ALA:HB3 | 1:16:A:TYR:HD1 | 15       | 0.11          |
| (1,56)  | 1:13:A:ALA:HB3 | 1:16:A:TYR:HD2 | 15       | 0.11          |
| (1,56)  | 1:13:A:ALA:HB1 | 1:16:A:TYR:HD1 | 17       | 0.11          |
| (1,56)  | 1:13:A:ALA:HB1 | 1:16:A:TYR:HD2 | 17       | 0.11          |
| (1,56)  | 1:13:A:ALA:HB2 | 1:16:A:TYR:HD1 | 17       | 0.11          |

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| Key    | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|--------|-----------------|----------------|----------|---------------|
| (1,56) | 1:13:A:ALA:HB2  | 1:16:A:TYR:HD2 | 17       | 0.11          |
| (1,56) | 1:13:A:ALA:HB3  | 1:16:A:TYR:HD1 | 17       | 0.11          |
| (1,56) | 1:13:A:ALA:HB3  | 1:16:A:TYR:HD2 | 17       | 0.11          |
| (1,54) | 1:13:A:ALA:HB1  | 1:13:A:ALA:H   | 8        | 0.11          |
| (1,54) | 1:13:A:ALA:HB2  | 1:13:A:ALA:H   | 8        | 0.11          |
| (1,54) | 1:13:A:ALA:HB3  | 1:13:A:ALA:H   | 8        | 0.11          |
| (1,54) | 1:13:A:ALA:HB1  | 1:13:A:ALA:H   | 14       | 0.11          |
| (1,54) | 1:13:A:ALA:HB2  | 1:13:A:ALA:H   | 14       | 0.11          |
| (1,54) | 1:13:A:ALA:HB3  | 1:13:A:ALA:H   | 14       | 0.11          |
| (1,54) | 1:13:A:ALA:HB1  | 1:13:A:ALA:H   | 19       | 0.11          |
| (1,54) | 1:13:A:ALA:HB2  | 1:13:A:ALA:H   | 19       | 0.11          |
| (1,54) | 1:13:A:ALA:HB3  | 1:13:A:ALA:H   | 19       | 0.11          |
| (1,54) | 1:13:A:ALA:HB1  | 1:13:A:ALA:H   | 20       | 0.11          |
| (1,54) | 1:13:A:ALA:HB2  | 1:13:A:ALA:H   | 20       | 0.11          |
| (1,54) | 1:13:A:ALA:HB3  | 1:13:A:ALA:H   | 20       | 0.11          |
| (1,51) | 1:13:A:ALA:HA   | 1:51:A:HIS:H   | 7        | 0.11          |
| (1,51) | 1:13:A:ALA:HA   | 1:51:A:HIS:H   | 15       | 0.11          |
| (1,51) | 1:13:A:ALA:HA   | 1:51:A:HIS:H   | 17       | 0.11          |
| (1,29) | 1:11:A:GLU:HG2  | 1:12:A:SER:H   | 2        | 0.11          |
| (1,29) | 1:11:A:GLU:HG3  | 1:12:A:SER:H   | 2        | 0.11          |
| (1,29) | 1:11:A:GLU:HG2  | 1:12:A:SER:H   | 3        | 0.11          |
| (1,29) | 1:11:A:GLU:HG3  | 1:12:A:SER:H   | 3        | 0.11          |
| (1,29) | 1:11:A:GLU:HG2  | 1:12:A:SER:H   | 5        | 0.11          |
| (1,29) | 1:11:A:GLU:HG3  | 1:12:A:SER:H   | 5        | 0.11          |
| (1,29) | 1:11:A:GLU:HG2  | 1:12:A:SER:H   | 6        | 0.11          |
| (1,29) | 1:11:A:GLU:HG3  | 1:12:A:SER:H   | 6        | 0.11          |
| (1,29) | 1:11:A:GLU:HG2  | 1:12:A:SER:H   | 12       | 0.11          |
| (1,29) | 1:11:A:GLU:HG3  | 1:12:A:SER:H   | 12       | 0.11          |
| (1,29) | 1:11:A:GLU:HG2  | 1:12:A:SER:H   | 14       | 0.11          |
| (1,29) | 1:11:A:GLU:HG3  | 1:12:A:SER:H   | 14       | 0.11          |
| (1,29) | 1:11:A:GLU:HG2  | 1:12:A:SER:H   | 15       | 0.11          |
| (1,29) | 1:11:A:GLU:HG3  | 1:12:A:SER:H   | 15       | 0.11          |
| (1,29) | 1:11:A:GLU:HG2  | 1:12:A:SER:H   | 16       | 0.11          |
| (1,29) | 1:11:A:GLU:HG3  | 1:12:A:SER:H   | 16       | 0.11          |
| (1,5)  | 1:10:A:THR:HG21 | 1:13:A:ALA:HA  | 1        | 0.11          |
| (1,5)  | 1:10:A:THR:HG22 | 1:13:A:ALA:HA  | 1        | 0.11          |
| (1,5)  | 1:10:A:THR:HG23 | 1:13:A:ALA:HA  | 1        | 0.11          |
| (1,5)  | 1:10:A:THR:HG21 | 1:13:A:ALA:HA  | 2        | 0.11          |
| (1,5)  | 1:10:A:THR:HG22 | 1:13:A:ALA:HA  | 2        | 0.11          |
| (1,5)  | 1:10:A:THR:HG23 | 1:13:A:ALA:HA  | 2        | 0.11          |
| (1,5)  | 1:10:A:THR:HG21 | 1:13:A:ALA:HA  | 3        | 0.11          |
| (1,5)  | 1:10:A:THR:HG22 | 1:13:A:ALA:HA  | 3        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,5)    | 1:10:A:THR:HG23 | 1:13:A:ALA:HA   | 3        | 0.11          |
| (1,1386) | 1:9:A:ARG:HA    | 1:54:A:HIS:HA   | 5        | 0.1           |
| (1,1386) | 1:9:A:ARG:HA    | 1:54:A:HIS:HA   | 6        | 0.1           |
| (1,1386) | 1:9:A:ARG:HA    | 1:54:A:HIS:HA   | 7        | 0.1           |
| (1,1342) | 1:90:A:ALA:HB1  | 1:90:A:ALA:H    | 3        | 0.1           |
| (1,1342) | 1:90:A:ALA:HB2  | 1:90:A:ALA:H    | 3        | 0.1           |
| (1,1342) | 1:90:A:ALA:HB3  | 1:90:A:ALA:H    | 3        | 0.1           |
| (1,1342) | 1:90:A:ALA:HB1  | 1:90:A:ALA:H    | 7        | 0.1           |
| (1,1342) | 1:90:A:ALA:HB2  | 1:90:A:ALA:H    | 7        | 0.1           |
| (1,1342) | 1:90:A:ALA:HB3  | 1:90:A:ALA:H    | 7        | 0.1           |
| (1,1342) | 1:90:A:ALA:HB1  | 1:90:A:ALA:H    | 13       | 0.1           |
| (1,1342) | 1:90:A:ALA:HB2  | 1:90:A:ALA:H    | 13       | 0.1           |
| (1,1342) | 1:90:A:ALA:HB3  | 1:90:A:ALA:H    | 13       | 0.1           |
| (1,1342) | 1:90:A:ALA:HB1  | 1:90:A:ALA:H    | 15       | 0.1           |
| (1,1342) | 1:90:A:ALA:HB2  | 1:90:A:ALA:H    | 15       | 0.1           |
| (1,1342) | 1:90:A:ALA:HB3  | 1:90:A:ALA:H    | 15       | 0.1           |
| (1,1342) | 1:90:A:ALA:HB1  | 1:90:A:ALA:H    | 18       | 0.1           |
| (1,1342) | 1:90:A:ALA:HB2  | 1:90:A:ALA:H    | 18       | 0.1           |
| (1,1342) | 1:90:A:ALA:HB3  | 1:90:A:ALA:H    | 18       | 0.1           |
| (1,1342) | 1:90:A:ALA:HB1  | 1:90:A:ALA:H    | 19       | 0.1           |
| (1,1342) | 1:90:A:ALA:HB2  | 1:90:A:ALA:H    | 19       | 0.1           |
| (1,1342) | 1:90:A:ALA:HB3  | 1:90:A:ALA:H    | 19       | 0.1           |
| (1,1315) | 1:87:A:LEU:HG   | 1:87:A:LEU:H    | 18       | 0.1           |
| (1,1309) | 1:87:A:LEU:HB2  | 1:87:A:LEU:H    | 11       | 0.1           |
| (1,1308) | 1:87:A:LEU:HB3  | 1:89:A:ILE:HA   | 10       | 0.1           |
| (1,1308) | 1:87:A:LEU:HB3  | 1:89:A:ILE:HA   | 15       | 0.1           |
| (1,1308) | 1:87:A:LEU:HB3  | 1:89:A:ILE:HA   | 16       | 0.1           |
| (1,1308) | 1:87:A:LEU:HB3  | 1:89:A:ILE:HA   | 17       | 0.1           |
| (1,1308) | 1:87:A:LEU:HB3  | 1:89:A:ILE:HA   | 19       | 0.1           |
| (1,1276) | 1:80:A:ARG:HG2  | 1:81:A:MET:H    | 6        | 0.1           |
| (1,1145) | 1:74:A:VAL:HB   | 1:76:A:ASP:H    | 19       | 0.1           |
| (1,1127) | 1:73:A:VAL:HG12 | 1:77:A:HIS:HD2  | 8        | 0.1           |
| (1,1127) | 1:73:A:VAL:HG12 | 1:77:A:HIS:HD2  | 11       | 0.1           |
| (1,1084) | 1:70:A:MET:H    | 1:71:A:GLN:H    | 14       | 0.1           |
| (1,1084) | 1:70:A:MET:H    | 1:71:A:GLN:H    | 18       | 0.1           |
| (1,1063) | 1:6:A:SER:H     | 1:58:A:ILE:HG21 | 1        | 0.1           |
| (1,1063) | 1:6:A:SER:H     | 1:58:A:ILE:HG22 | 1        | 0.1           |
| (1,1063) | 1:6:A:SER:H     | 1:58:A:ILE:HG23 | 1        | 0.1           |
| (1,1063) | 1:6:A:SER:H     | 1:58:A:ILE:HG21 | 5        | 0.1           |
| (1,1063) | 1:6:A:SER:H     | 1:58:A:ILE:HG22 | 5        | 0.1           |
| (1,1063) | 1:6:A:SER:H     | 1:58:A:ILE:HG23 | 5        | 0.1           |
| (1,1063) | 1:6:A:SER:H     | 1:58:A:ILE:HG21 | 9        | 0.1           |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1063) | 1:6:A:SER:H    | 1:58:A:ILE:HG22 | 9        | 0.1           |
| (1,1063) | 1:6:A:SER:H    | 1:58:A:ILE:HG23 | 9        | 0.1           |
| (1,1063) | 1:6:A:SER:H    | 1:58:A:ILE:HG21 | 19       | 0.1           |
| (1,1063) | 1:6:A:SER:H    | 1:58:A:ILE:HG22 | 19       | 0.1           |
| (1,1063) | 1:6:A:SER:H    | 1:58:A:ILE:HG23 | 19       | 0.1           |
| (1,1014) | 1:68:A:ALA:HA  | 1:71:A:GLN:HA   | 5        | 0.1           |
| (1,969)  | 1:64:A:GLU:H   | 1:65:A:ASP:H    | 7        | 0.1           |
| (1,964)  | 1:64:A:GLU:HG2 | 1:67:A:LEU:HG   | 2        | 0.1           |
| (1,964)  | 1:64:A:GLU:HG3 | 1:67:A:LEU:HG   | 2        | 0.1           |
| (1,964)  | 1:64:A:GLU:HG2 | 1:67:A:LEU:HG   | 4        | 0.1           |
| (1,964)  | 1:64:A:GLU:HG3 | 1:67:A:LEU:HG   | 4        | 0.1           |
| (1,964)  | 1:64:A:GLU:HG2 | 1:67:A:LEU:HG   | 5        | 0.1           |
| (1,964)  | 1:64:A:GLU:HG3 | 1:67:A:LEU:HG   | 5        | 0.1           |
| (1,964)  | 1:64:A:GLU:HG2 | 1:67:A:LEU:HG   | 9        | 0.1           |
| (1,964)  | 1:64:A:GLU:HG3 | 1:67:A:LEU:HG   | 9        | 0.1           |
| (1,964)  | 1:64:A:GLU:HG2 | 1:67:A:LEU:HG   | 10       | 0.1           |
| (1,964)  | 1:64:A:GLU:HG3 | 1:67:A:LEU:HG   | 10       | 0.1           |
| (1,964)  | 1:64:A:GLU:HG2 | 1:67:A:LEU:HG   | 11       | 0.1           |
| (1,964)  | 1:64:A:GLU:HG3 | 1:67:A:LEU:HG   | 11       | 0.1           |
| (1,964)  | 1:64:A:GLU:HG2 | 1:67:A:LEU:HG   | 17       | 0.1           |
| (1,964)  | 1:64:A:GLU:HG3 | 1:67:A:LEU:HG   | 17       | 0.1           |
| (1,964)  | 1:64:A:GLU:HG2 | 1:67:A:LEU:HG   | 18       | 0.1           |
| (1,964)  | 1:64:A:GLU:HG3 | 1:67:A:LEU:HG   | 18       | 0.1           |
| (1,938)  | 1:63:A:ASP:H   | 1:66:A:SER:HA   | 8        | 0.1           |
| (1,938)  | 1:63:A:ASP:H   | 1:66:A:SER:HA   | 10       | 0.1           |
| (1,932)  | 1:63:A:ASP:HB2 | 1:66:A:SER:H    | 15       | 0.1           |
| (1,932)  | 1:63:A:ASP:HB3 | 1:66:A:SER:H    | 15       | 0.1           |
| (1,914)  | 1:61:A:SER:HB2 | 1:67:A:LEU:HA   | 10       | 0.1           |
| (1,914)  | 1:61:A:SER:HB3 | 1:67:A:LEU:HA   | 10       | 0.1           |
| (1,914)  | 1:61:A:SER:HB2 | 1:67:A:LEU:HA   | 14       | 0.1           |
| (1,914)  | 1:61:A:SER:HB3 | 1:67:A:LEU:HA   | 14       | 0.1           |
| (1,914)  | 1:61:A:SER:HB2 | 1:67:A:LEU:HA   | 19       | 0.1           |
| (1,914)  | 1:61:A:SER:HB3 | 1:67:A:LEU:HA   | 19       | 0.1           |
| (1,774)  | 1:51:A:HIS:H   | 1:52:A:PRO:HD2  | 9        | 0.1           |
| (1,774)  | 1:51:A:HIS:H   | 1:52:A:PRO:HD2  | 11       | 0.1           |
| (1,774)  | 1:51:A:HIS:H   | 1:52:A:PRO:HD2  | 12       | 0.1           |
| (1,773)  | 1:51:A:HIS:H   | 1:52:A:PRO:HD3  | 6        | 0.1           |
| (1,739)  | 1:4:A:SER:HB2  | 1:59:A:LEU:HB2  | 10       | 0.1           |
| (1,739)  | 1:4:A:SER:HB2  | 1:59:A:LEU:HB3  | 10       | 0.1           |
| (1,739)  | 1:4:A:SER:HB3  | 1:59:A:LEU:HB2  | 10       | 0.1           |
| (1,739)  | 1:4:A:SER:HB3  | 1:59:A:LEU:HB3  | 10       | 0.1           |
| (1,739)  | 1:4:A:SER:HB2  | 1:59:A:LEU:HB2  | 15       | 0.1           |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,739) | 1:4:A:SER:HB2  | 1:59:A:LEU:HB3  | 15       | 0.1           |
| (1,739) | 1:4:A:SER:HB3  | 1:59:A:LEU:HB2  | 15       | 0.1           |
| (1,739) | 1:4:A:SER:HB3  | 1:59:A:LEU:HB3  | 15       | 0.1           |
| (1,738) | 1:4:A:SER:HB2  | 1:94:A:ALA:H    | 1        | 0.1           |
| (1,738) | 1:4:A:SER:HB2  | 1:94:A:ALA:H    | 14       | 0.1           |
| (1,738) | 1:4:A:SER:HB2  | 1:94:A:ALA:H    | 18       | 0.1           |
| (1,724) | 1:49:A:LEU:H   | 1:57:A:MET:HA   | 5        | 0.1           |
| (1,703) | 1:48:A:LEU:HB2 | 1:48:A:LEU:HD11 | 7        | 0.1           |
| (1,703) | 1:48:A:LEU:HB2 | 1:48:A:LEU:HD12 | 7        | 0.1           |
| (1,703) | 1:48:A:LEU:HB2 | 1:48:A:LEU:HD13 | 7        | 0.1           |
| (1,703) | 1:48:A:LEU:HB2 | 1:48:A:LEU:HD21 | 7        | 0.1           |
| (1,703) | 1:48:A:LEU:HB2 | 1:48:A:LEU:HD22 | 7        | 0.1           |
| (1,703) | 1:48:A:LEU:HB2 | 1:48:A:LEU:HD23 | 7        | 0.1           |
| (1,703) | 1:48:A:LEU:HB3 | 1:48:A:LEU:HD11 | 7        | 0.1           |
| (1,703) | 1:48:A:LEU:HB3 | 1:48:A:LEU:HD12 | 7        | 0.1           |
| (1,703) | 1:48:A:LEU:HB3 | 1:48:A:LEU:HD13 | 7        | 0.1           |
| (1,703) | 1:48:A:LEU:HB3 | 1:48:A:LEU:HD21 | 7        | 0.1           |
| (1,703) | 1:48:A:LEU:HB3 | 1:48:A:LEU:HD22 | 7        | 0.1           |
| (1,703) | 1:48:A:LEU:HB3 | 1:48:A:LEU:HD23 | 7        | 0.1           |
| (1,703) | 1:48:A:LEU:HB2 | 1:48:A:LEU:HD11 | 10       | 0.1           |
| (1,703) | 1:48:A:LEU:HB2 | 1:48:A:LEU:HD12 | 10       | 0.1           |
| (1,703) | 1:48:A:LEU:HB2 | 1:48:A:LEU:HD13 | 10       | 0.1           |
| (1,703) | 1:48:A:LEU:HB2 | 1:48:A:LEU:HD21 | 10       | 0.1           |
| (1,703) | 1:48:A:LEU:HB2 | 1:48:A:LEU:HD22 | 10       | 0.1           |
| (1,703) | 1:48:A:LEU:HB2 | 1:48:A:LEU:HD23 | 10       | 0.1           |
| (1,703) | 1:48:A:LEU:HB3 | 1:48:A:LEU:HD11 | 10       | 0.1           |
| (1,703) | 1:48:A:LEU:HB3 | 1:48:A:LEU:HD12 | 10       | 0.1           |
| (1,703) | 1:48:A:LEU:HB3 | 1:48:A:LEU:HD13 | 10       | 0.1           |
| (1,703) | 1:48:A:LEU:HB3 | 1:48:A:LEU:HD21 | 10       | 0.1           |
| (1,703) | 1:48:A:LEU:HB3 | 1:48:A:LEU:HD22 | 10       | 0.1           |
| (1,703) | 1:48:A:LEU:HB3 | 1:48:A:LEU:HD23 | 10       | 0.1           |
| (1,703) | 1:48:A:LEU:HB2 | 1:48:A:LEU:HD11 | 17       | 0.1           |
| (1,703) | 1:48:A:LEU:HB2 | 1:48:A:LEU:HD12 | 17       | 0.1           |
| (1,703) | 1:48:A:LEU:HB2 | 1:48:A:LEU:HD13 | 17       | 0.1           |
| (1,703) | 1:48:A:LEU:HB2 | 1:48:A:LEU:HD21 | 17       | 0.1           |
| (1,703) | 1:48:A:LEU:HB2 | 1:48:A:LEU:HD22 | 17       | 0.1           |
| (1,703) | 1:48:A:LEU:HB2 | 1:48:A:LEU:HD23 | 17       | 0.1           |
| (1,703) | 1:48:A:LEU:HB3 | 1:48:A:LEU:HD11 | 17       | 0.1           |
| (1,703) | 1:48:A:LEU:HB3 | 1:48:A:LEU:HD12 | 17       | 0.1           |
| (1,703) | 1:48:A:LEU:HB3 | 1:48:A:LEU:HD13 | 17       | 0.1           |
| (1,703) | 1:48:A:LEU:HB3 | 1:48:A:LEU:HD21 | 17       | 0.1           |
| (1,703) | 1:48:A:LEU:HB3 | 1:48:A:LEU:HD22 | 17       | 0.1           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,703) | 1:48:A:LEU:HB3  | 1:48:A:LEU:HD23 | 17       | 0.1           |
| (1,688) | 1:47:A:GLU:HA   | 1:47:A:GLU:HG2  | 18       | 0.1           |
| (1,688) | 1:47:A:GLU:HA   | 1:47:A:GLU:HG3  | 18       | 0.1           |
| (1,673) | 1:45:A:ASN:H    | 1:70:A:MET:HB3  | 4        | 0.1           |
| (1,651) | 1:44:A:SER:HB3  | 1:61:A:SER:HA   | 1        | 0.1           |
| (1,651) | 1:44:A:SER:HB3  | 1:61:A:SER:HA   | 20       | 0.1           |
| (1,601) | 1:3:A:ARG:HG2   | 1:61:A:SER:H    | 5        | 0.1           |
| (1,601) | 1:3:A:ARG:HG2   | 1:61:A:SER:H    | 13       | 0.1           |
| (1,571) | 1:39:A:ILE:H    | 1:46:A:CYS:H    | 7        | 0.1           |
| (1,557) | 1:39:A:ILE:HG13 | 1:39:A:ILE:H    | 3        | 0.1           |
| (1,557) | 1:39:A:ILE:HG13 | 1:39:A:ILE:H    | 14       | 0.1           |
| (1,542) | 1:38:A:PHE:HE1  | 1:45:A:ASN:HB2  | 5        | 0.1           |
| (1,542) | 1:38:A:PHE:HE1  | 1:45:A:ASN:HB3  | 5        | 0.1           |
| (1,542) | 1:38:A:PHE:HE2  | 1:45:A:ASN:HB2  | 5        | 0.1           |
| (1,542) | 1:38:A:PHE:HE2  | 1:45:A:ASN:HB3  | 5        | 0.1           |
| (1,542) | 1:38:A:PHE:HE1  | 1:45:A:ASN:HB2  | 18       | 0.1           |
| (1,542) | 1:38:A:PHE:HE1  | 1:45:A:ASN:HB3  | 18       | 0.1           |
| (1,542) | 1:38:A:PHE:HE2  | 1:45:A:ASN:HB2  | 18       | 0.1           |
| (1,542) | 1:38:A:PHE:HE2  | 1:45:A:ASN:HB3  | 18       | 0.1           |
| (1,539) | 1:38:A:PHE:HD1  | 1:48:A:LEU:H    | 7        | 0.1           |
| (1,539) | 1:38:A:PHE:HD2  | 1:48:A:LEU:H    | 7        | 0.1           |
| (1,534) | 1:38:A:PHE:HD1  | 1:45:A:ASN:HB2  | 4        | 0.1           |
| (1,534) | 1:38:A:PHE:HD1  | 1:45:A:ASN:HB3  | 4        | 0.1           |
| (1,534) | 1:38:A:PHE:HD2  | 1:45:A:ASN:HB2  | 4        | 0.1           |
| (1,534) | 1:38:A:PHE:HD2  | 1:45:A:ASN:HB3  | 4        | 0.1           |
| (1,521) | 1:38:A:PHE:HA   | 1:46:A:CYS:H    | 4        | 0.1           |
| (1,521) | 1:38:A:PHE:HA   | 1:46:A:CYS:H    | 5        | 0.1           |
| (1,521) | 1:38:A:PHE:HA   | 1:46:A:CYS:H    | 20       | 0.1           |
| (1,493) | 1:36:A:ARG:HA   | 1:49:A:LEU:HA   | 11       | 0.1           |
| (1,482) | 1:35:A:GLU:HB2  | 1:36:A:ARG:H    | 20       | 0.1           |
| (1,472) | 1:34:A:PRO:HB3  | 1:35:A:GLU:H    | 2        | 0.1           |
| (1,472) | 1:34:A:PRO:HB3  | 1:35:A:GLU:H    | 7        | 0.1           |
| (1,472) | 1:34:A:PRO:HB3  | 1:35:A:GLU:H    | 13       | 0.1           |
| (1,472) | 1:34:A:PRO:HB3  | 1:35:A:GLU:H    | 16       | 0.1           |
| (1,437) | 1:32:A:LEU:HB3  | 1:32:A:LEU:H    | 1        | 0.1           |
| (1,437) | 1:32:A:LEU:HB3  | 1:32:A:LEU:H    | 15       | 0.1           |
| (1,398) | 1:30:A:VAL:HA   | 1:30:A:VAL:HG11 | 9        | 0.1           |
| (1,398) | 1:30:A:VAL:HA   | 1:30:A:VAL:HG12 | 9        | 0.1           |
| (1,398) | 1:30:A:VAL:HA   | 1:30:A:VAL:HG13 | 9        | 0.1           |
| (1,398) | 1:30:A:VAL:HA   | 1:30:A:VAL:HG11 | 11       | 0.1           |
| (1,398) | 1:30:A:VAL:HA   | 1:30:A:VAL:HG12 | 11       | 0.1           |
| (1,398) | 1:30:A:VAL:HA   | 1:30:A:VAL:HG13 | 11       | 0.1           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,398) | 1:30:A:VAL:HA   | 1:30:A:VAL:HG11 | 12       | 0.1           |
| (1,398) | 1:30:A:VAL:HA   | 1:30:A:VAL:HG12 | 12       | 0.1           |
| (1,398) | 1:30:A:VAL:HA   | 1:30:A:VAL:HG13 | 12       | 0.1           |
| (1,398) | 1:30:A:VAL:HA   | 1:30:A:VAL:HG11 | 14       | 0.1           |
| (1,398) | 1:30:A:VAL:HA   | 1:30:A:VAL:HG12 | 14       | 0.1           |
| (1,398) | 1:30:A:VAL:HA   | 1:30:A:VAL:HG13 | 14       | 0.1           |
| (1,398) | 1:30:A:VAL:HA   | 1:30:A:VAL:HG11 | 15       | 0.1           |
| (1,398) | 1:30:A:VAL:HA   | 1:30:A:VAL:HG12 | 15       | 0.1           |
| (1,398) | 1:30:A:VAL:HA   | 1:30:A:VAL:HG13 | 15       | 0.1           |
| (1,398) | 1:30:A:VAL:HA   | 1:30:A:VAL:HG11 | 19       | 0.1           |
| (1,398) | 1:30:A:VAL:HA   | 1:30:A:VAL:HG12 | 19       | 0.1           |
| (1,398) | 1:30:A:VAL:HA   | 1:30:A:VAL:HG13 | 19       | 0.1           |
| (1,394) | 1:2:A:PHE:H     | 1:62:A:PRO:HD2  | 13       | 0.1           |
| (1,394) | 1:2:A:PHE:H     | 1:62:A:PRO:HD3  | 13       | 0.1           |
| (1,394) | 1:2:A:PHE:H     | 1:62:A:PRO:HD2  | 15       | 0.1           |
| (1,394) | 1:2:A:PHE:H     | 1:62:A:PRO:HD3  | 15       | 0.1           |
| (1,394) | 1:2:A:PHE:H     | 1:62:A:PRO:HD2  | 17       | 0.1           |
| (1,394) | 1:2:A:PHE:H     | 1:62:A:PRO:HD3  | 17       | 0.1           |
| (1,372) | 1:29:A:GLU:H    | 1:41:A:PHE:HA   | 2        | 0.1           |
| (1,372) | 1:29:A:GLU:H    | 1:41:A:PHE:HA   | 9        | 0.1           |
| (1,372) | 1:29:A:GLU:H    | 1:41:A:PHE:HA   | 20       | 0.1           |
| (1,335) | 1:28:A:PHE:HA   | 1:30:A:VAL:HG21 | 2        | 0.1           |
| (1,335) | 1:28:A:PHE:HA   | 1:30:A:VAL:HG22 | 2        | 0.1           |
| (1,335) | 1:28:A:PHE:HA   | 1:30:A:VAL:HG23 | 2        | 0.1           |
| (1,284) | 1:24:A:TRP:HA   | 1:25:A:GLY:H    | 10       | 0.1           |
| (1,284) | 1:24:A:TRP:HA   | 1:25:A:GLY:H    | 18       | 0.1           |
| (1,283) | 1:23:A:HIS:H    | 1:30:A:VAL:HG21 | 7        | 0.1           |
| (1,283) | 1:23:A:HIS:H    | 1:30:A:VAL:HG22 | 7        | 0.1           |
| (1,283) | 1:23:A:HIS:H    | 1:30:A:VAL:HG23 | 7        | 0.1           |
| (1,283) | 1:23:A:HIS:H    | 1:30:A:VAL:HG21 | 17       | 0.1           |
| (1,283) | 1:23:A:HIS:H    | 1:30:A:VAL:HG22 | 17       | 0.1           |
| (1,283) | 1:23:A:HIS:H    | 1:30:A:VAL:HG23 | 17       | 0.1           |
| (1,199) | 1:1:A:MET:HA    | 1:62:A:PRO:HA   | 9        | 0.1           |
| (1,191) | 1:19:A:ARG:HG2  | 1:19:A:ARG:H    | 2        | 0.1           |
| (1,191) | 1:19:A:ARG:HG3  | 1:19:A:ARG:H    | 2        | 0.1           |
| (1,191) | 1:19:A:ARG:HG2  | 1:19:A:ARG:H    | 13       | 0.1           |
| (1,191) | 1:19:A:ARG:HG3  | 1:19:A:ARG:H    | 13       | 0.1           |
| (1,176) | 1:18:A:ASN:H    | 1:19:A:ARG:H    | 3        | 0.1           |
| (1,176) | 1:18:A:ASN:H    | 1:19:A:ARG:H    | 12       | 0.1           |
| (1,176) | 1:18:A:ASN:H    | 1:19:A:ARG:H    | 15       | 0.1           |
| (1,160) | 1:17:A:VAL:HG21 | 1:36:A:ARG:H    | 15       | 0.1           |
| (1,160) | 1:17:A:VAL:HG22 | 1:36:A:ARG:H    | 15       | 0.1           |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,160) | 1:17:A:VAL:HG23 | 1:36:A:ARG:H   | 15       | 0.1           |
| (1,160) | 1:17:A:VAL:HG21 | 1:36:A:ARG:H   | 19       | 0.1           |
| (1,160) | 1:17:A:VAL:HG22 | 1:36:A:ARG:H   | 19       | 0.1           |
| (1,160) | 1:17:A:VAL:HG23 | 1:36:A:ARG:H   | 19       | 0.1           |
| (1,151) | 1:17:A:VAL:HG11 | 1:18:A:ASN:H   | 5        | 0.1           |
| (1,151) | 1:17:A:VAL:HG12 | 1:18:A:ASN:H   | 5        | 0.1           |
| (1,151) | 1:17:A:VAL:HG13 | 1:18:A:ASN:H   | 5        | 0.1           |
| (1,151) | 1:17:A:VAL:HG11 | 1:18:A:ASN:H   | 12       | 0.1           |
| (1,151) | 1:17:A:VAL:HG12 | 1:18:A:ASN:H   | 12       | 0.1           |
| (1,151) | 1:17:A:VAL:HG13 | 1:18:A:ASN:H   | 12       | 0.1           |
| (1,151) | 1:17:A:VAL:HG11 | 1:18:A:ASN:H   | 14       | 0.1           |
| (1,151) | 1:17:A:VAL:HG12 | 1:18:A:ASN:H   | 14       | 0.1           |
| (1,151) | 1:17:A:VAL:HG13 | 1:18:A:ASN:H   | 14       | 0.1           |
| (1,134) | 1:16:A:TYR:H    | 1:17:A:VAL:HB  | 10       | 0.1           |
| (1,116) | 1:15:A:ARG:HG2  | 1:16:A:TYR:H   | 7        | 0.1           |
| (1,116) | 1:15:A:ARG:HG3  | 1:16:A:TYR:H   | 7        | 0.1           |
| (1,96)  | 1:15:A:ARG:HA   | 1:19:A:ARG:H   | 11       | 0.1           |
| (1,85)  | 1:14:A:ALA:HB1  | 1:50:A:ALA:HA  | 1        | 0.1           |
| (1,85)  | 1:14:A:ALA:HB2  | 1:50:A:ALA:HA  | 1        | 0.1           |
| (1,85)  | 1:14:A:ALA:HB3  | 1:50:A:ALA:HA  | 1        | 0.1           |
| (1,85)  | 1:14:A:ALA:HB1  | 1:50:A:ALA:HA  | 8        | 0.1           |
| (1,85)  | 1:14:A:ALA:HB2  | 1:50:A:ALA:HA  | 8        | 0.1           |
| (1,85)  | 1:14:A:ALA:HB3  | 1:50:A:ALA:HA  | 8        | 0.1           |
| (1,85)  | 1:14:A:ALA:HB1  | 1:50:A:ALA:HA  | 19       | 0.1           |
| (1,85)  | 1:14:A:ALA:HB2  | 1:50:A:ALA:HA  | 19       | 0.1           |
| (1,85)  | 1:14:A:ALA:HB3  | 1:50:A:ALA:HA  | 19       | 0.1           |
| (1,71)  | 1:14:A:ALA:HA   | 1:14:A:ALA:H   | 4        | 0.1           |
| (1,71)  | 1:14:A:ALA:HA   | 1:14:A:ALA:H   | 11       | 0.1           |
| (1,71)  | 1:14:A:ALA:HA   | 1:14:A:ALA:H   | 12       | 0.1           |
| (1,71)  | 1:14:A:ALA:HA   | 1:14:A:ALA:H   | 14       | 0.1           |
| (1,56)  | 1:13:A:ALA:HB1  | 1:16:A:TYR:HD1 | 1        | 0.1           |
| (1,56)  | 1:13:A:ALA:HB1  | 1:16:A:TYR:HD2 | 1        | 0.1           |
| (1,56)  | 1:13:A:ALA:HB2  | 1:16:A:TYR:HD1 | 1        | 0.1           |
| (1,56)  | 1:13:A:ALA:HB2  | 1:16:A:TYR:HD2 | 1        | 0.1           |
| (1,56)  | 1:13:A:ALA:HB3  | 1:16:A:TYR:HD1 | 1        | 0.1           |
| (1,56)  | 1:13:A:ALA:HB3  | 1:16:A:TYR:HD2 | 1        | 0.1           |
| (1,56)  | 1:13:A:ALA:HB1  | 1:16:A:TYR:HD1 | 5        | 0.1           |
| (1,56)  | 1:13:A:ALA:HB1  | 1:16:A:TYR:HD2 | 5        | 0.1           |
| (1,56)  | 1:13:A:ALA:HB2  | 1:16:A:TYR:HD1 | 5        | 0.1           |
| (1,56)  | 1:13:A:ALA:HB2  | 1:16:A:TYR:HD2 | 5        | 0.1           |
| (1,56)  | 1:13:A:ALA:HB3  | 1:16:A:TYR:HD1 | 5        | 0.1           |
| (1,56)  | 1:13:A:ALA:HB3  | 1:16:A:TYR:HD2 | 5        | 0.1           |

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| Key    | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|--------|----------------|----------------|----------|---------------|
| (1,56) | 1:13:A:ALA:HB1 | 1:16:A:TYR:HD1 | 7        | 0.1           |
| (1,56) | 1:13:A:ALA:HB1 | 1:16:A:TYR:HD2 | 7        | 0.1           |
| (1,56) | 1:13:A:ALA:HB2 | 1:16:A:TYR:HD1 | 7        | 0.1           |
| (1,56) | 1:13:A:ALA:HB2 | 1:16:A:TYR:HD2 | 7        | 0.1           |
| (1,56) | 1:13:A:ALA:HB3 | 1:16:A:TYR:HD1 | 7        | 0.1           |
| (1,56) | 1:13:A:ALA:HB3 | 1:16:A:TYR:HD2 | 7        | 0.1           |
| (1,56) | 1:13:A:ALA:HB1 | 1:16:A:TYR:HD1 | 19       | 0.1           |
| (1,56) | 1:13:A:ALA:HB1 | 1:16:A:TYR:HD2 | 19       | 0.1           |
| (1,56) | 1:13:A:ALA:HB2 | 1:16:A:TYR:HD1 | 19       | 0.1           |
| (1,56) | 1:13:A:ALA:HB2 | 1:16:A:TYR:HD2 | 19       | 0.1           |
| (1,56) | 1:13:A:ALA:HB3 | 1:16:A:TYR:HD1 | 19       | 0.1           |
| (1,56) | 1:13:A:ALA:HB3 | 1:16:A:TYR:HD2 | 19       | 0.1           |
| (1,54) | 1:13:A:ALA:HB1 | 1:13:A:ALA:H   | 4        | 0.1           |
| (1,54) | 1:13:A:ALA:HB2 | 1:13:A:ALA:H   | 4        | 0.1           |
| (1,54) | 1:13:A:ALA:HB3 | 1:13:A:ALA:H   | 4        | 0.1           |
| (1,54) | 1:13:A:ALA:HB1 | 1:13:A:ALA:H   | 9        | 0.1           |
| (1,54) | 1:13:A:ALA:HB2 | 1:13:A:ALA:H   | 9        | 0.1           |
| (1,54) | 1:13:A:ALA:HB3 | 1:13:A:ALA:H   | 9        | 0.1           |
| (1,54) | 1:13:A:ALA:HB1 | 1:13:A:ALA:H   | 10       | 0.1           |
| (1,54) | 1:13:A:ALA:HB2 | 1:13:A:ALA:H   | 10       | 0.1           |
| (1,54) | 1:13:A:ALA:HB3 | 1:13:A:ALA:H   | 10       | 0.1           |
| (1,54) | 1:13:A:ALA:HB1 | 1:13:A:ALA:H   | 17       | 0.1           |
| (1,54) | 1:13:A:ALA:HB2 | 1:13:A:ALA:H   | 17       | 0.1           |
| (1,54) | 1:13:A:ALA:HB3 | 1:13:A:ALA:H   | 17       | 0.1           |
| (1,51) | 1:13:A:ALA:HA  | 1:51:A:HIS:H   | 1        | 0.1           |
| (1,51) | 1:13:A:ALA:HA  | 1:51:A:HIS:H   | 2        | 0.1           |
| (1,51) | 1:13:A:ALA:HA  | 1:51:A:HIS:H   | 3        | 0.1           |
| (1,51) | 1:13:A:ALA:HA  | 1:51:A:HIS:H   | 4        | 0.1           |
| (1,51) | 1:13:A:ALA:HA  | 1:51:A:HIS:H   | 5        | 0.1           |
| (1,51) | 1:13:A:ALA:HA  | 1:51:A:HIS:H   | 8        | 0.1           |
| (1,51) | 1:13:A:ALA:HA  | 1:51:A:HIS:H   | 9        | 0.1           |
| (1,51) | 1:13:A:ALA:HA  | 1:51:A:HIS:H   | 10       | 0.1           |
| (1,51) | 1:13:A:ALA:HA  | 1:51:A:HIS:H   | 12       | 0.1           |
| (1,51) | 1:13:A:ALA:HA  | 1:51:A:HIS:H   | 18       | 0.1           |
| (1,51) | 1:13:A:ALA:HA  | 1:51:A:HIS:H   | 19       | 0.1           |
| (1,51) | 1:13:A:ALA:HA  | 1:51:A:HIS:H   | 20       | 0.1           |
| (1,29) | 1:11:A:GLU:HG2 | 1:12:A:SER:H   | 1        | 0.1           |
| (1,29) | 1:11:A:GLU:HG3 | 1:12:A:SER:H   | 1        | 0.1           |
| (1,29) | 1:11:A:GLU:HG2 | 1:12:A:SER:H   | 4        | 0.1           |
| (1,29) | 1:11:A:GLU:HG3 | 1:12:A:SER:H   | 4        | 0.1           |
| (1,29) | 1:11:A:GLU:HG2 | 1:12:A:SER:H   | 7        | 0.1           |
| (1,29) | 1:11:A:GLU:HG3 | 1:12:A:SER:H   | 7        | 0.1           |

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| Key    | Atom-1         | Atom-2       | Model ID | Violation (Å) |
|--------|----------------|--------------|----------|---------------|
| (1,29) | 1:11:A:GLU:HG2 | 1:12:A:SER:H | 8        | 0.1           |
| (1,29) | 1:11:A:GLU:HG3 | 1:12:A:SER:H | 8        | 0.1           |
| (1,29) | 1:11:A:GLU:HG2 | 1:12:A:SER:H | 9        | 0.1           |
| (1,29) | 1:11:A:GLU:HG3 | 1:12:A:SER:H | 9        | 0.1           |
| (1,29) | 1:11:A:GLU:HG2 | 1:12:A:SER:H | 10       | 0.1           |
| (1,29) | 1:11:A:GLU:HG3 | 1:12:A:SER:H | 10       | 0.1           |
| (1,29) | 1:11:A:GLU:HG2 | 1:12:A:SER:H | 11       | 0.1           |
| (1,29) | 1:11:A:GLU:HG3 | 1:12:A:SER:H | 11       | 0.1           |
| (1,29) | 1:11:A:GLU:HG2 | 1:12:A:SER:H | 13       | 0.1           |
| (1,29) | 1:11:A:GLU:HG3 | 1:12:A:SER:H | 13       | 0.1           |
| (1,29) | 1:11:A:GLU:HG2 | 1:12:A:SER:H | 17       | 0.1           |
| (1,29) | 1:11:A:GLU:HG3 | 1:12:A:SER:H | 17       | 0.1           |

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

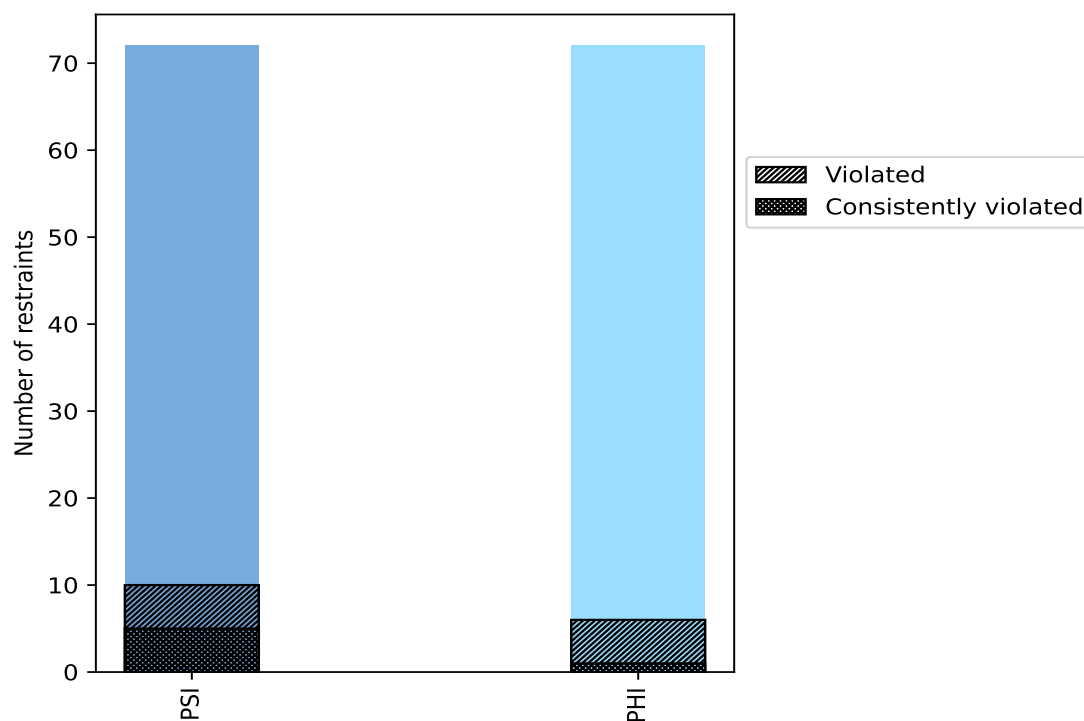
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PSI        | 72    | 50.0           | 10                    | 13.9           | 6.9            | 5                                  | 6.9            | 3.5            |
| PHI        | 72    | 50.0           | 6                     | 8.3            | 4.2            | 1                                  | 1.4            | 0.7            |
| Total      | 144   | 100.0          | 16                    | 11.1           | 11.1           | 6                                  | 4.2            | 4.2            |

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

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



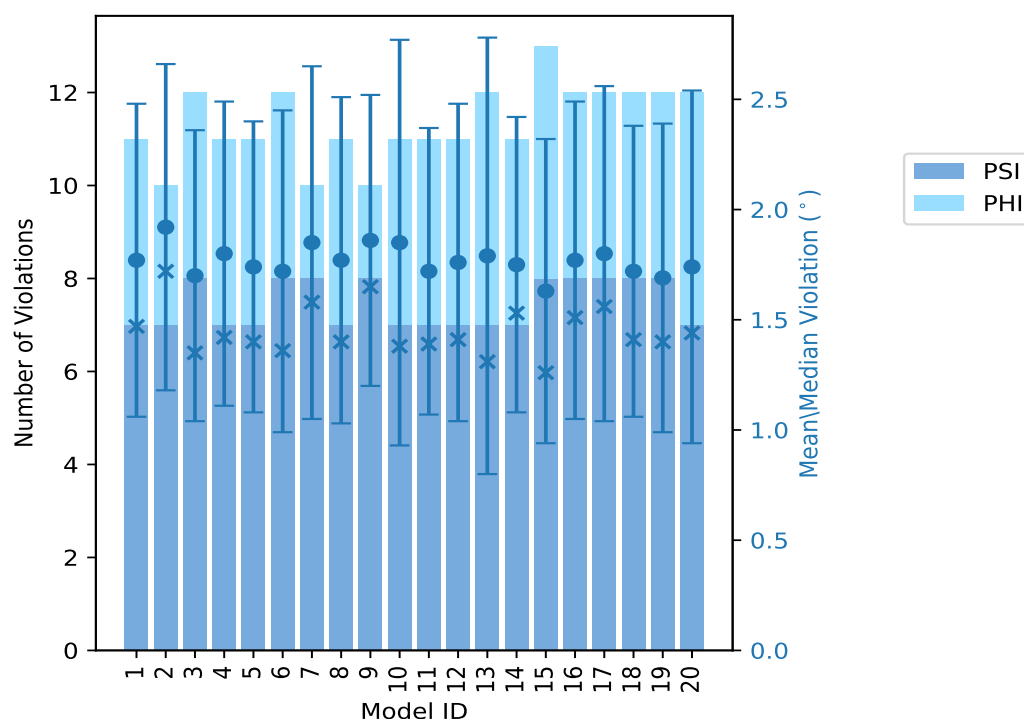
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PSI                  | PHI | Total |          |         |        |            |
| 1        | 7                    | 4   | 11    | 1.77     | 3.12    | 0.71   | 1.47       |
| 2        | 7                    | 3   | 10    | 1.92     | 3.29    | 0.74   | 1.72       |
| 3        | 8                    | 4   | 12    | 1.7      | 3.02    | 0.66   | 1.35       |
| 4        | 7                    | 4   | 11    | 1.8      | 3.19    | 0.69   | 1.42       |
| 5        | 7                    | 4   | 11    | 1.74     | 2.91    | 0.66   | 1.4        |
| 6        | 8                    | 4   | 12    | 1.72     | 3.28    | 0.73   | 1.36       |
| 7        | 8                    | 2   | 10    | 1.85     | 3.4     | 0.8    | 1.58       |
| 8        | 7                    | 4   | 11    | 1.77     | 3.25    | 0.74   | 1.4        |
| 9        | 8                    | 2   | 10    | 1.86     | 3.09    | 0.66   | 1.65       |
| 10       | 7                    | 4   | 11    | 1.85     | 3.67    | 0.92   | 1.38       |
| 11       | 7                    | 4   | 11    | 1.72     | 2.97    | 0.65   | 1.39       |
| 12       | 7                    | 4   | 11    | 1.76     | 3.15    | 0.72   | 1.41       |
| 13       | 7                    | 5   | 12    | 1.79     | 3.87    | 0.99   | 1.31       |
| 14       | 7                    | 4   | 11    | 1.75     | 2.96    | 0.67   | 1.53       |
| 15       | 8                    | 5   | 13    | 1.63     | 3.07    | 0.69   | 1.26       |
| 16       | 8                    | 4   | 12    | 1.77     | 3.28    | 0.72   | 1.51       |
| 17       | 8                    | 4   | 12    | 1.8      | 3.39    | 0.76   | 1.56       |
| 18       | 8                    | 4   | 12    | 1.72     | 3.1     | 0.66   | 1.41       |
| 19       | 8                    | 4   | 12    | 1.69     | 3.18    | 0.7    | 1.4        |
| 20       | 7                    | 5   | 12    | 1.74     | 3.37    | 0.8    | 1.44       |

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



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

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

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

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

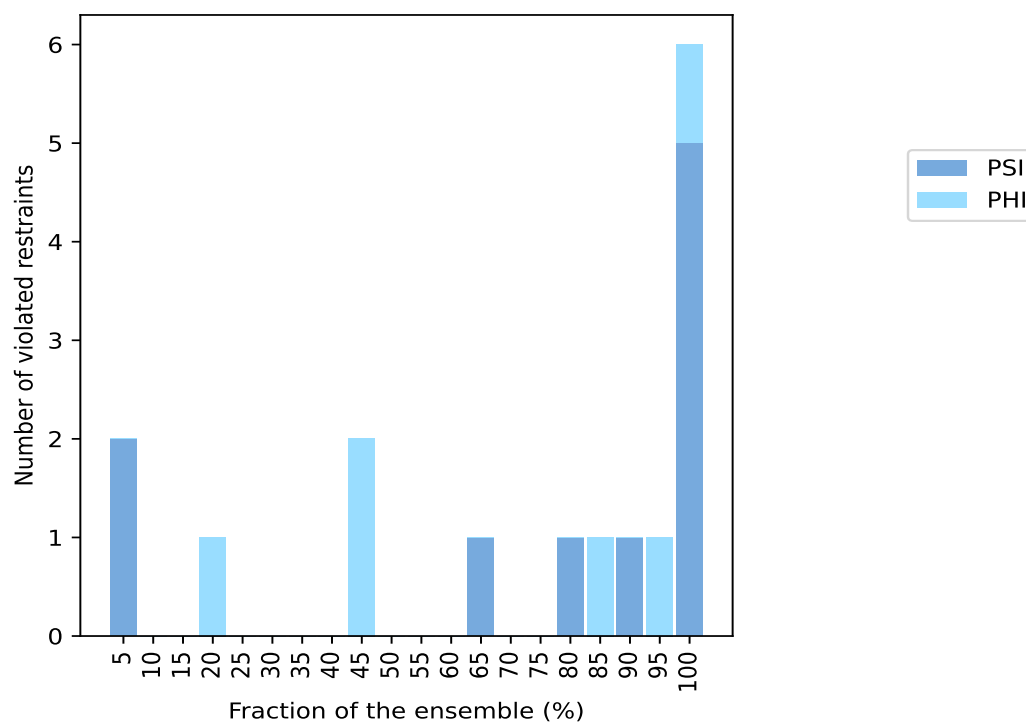
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %     |
| 0                             | 0   | 0     | 12                       | 60.0  |
| 1                             | 0   | 1     | 13                       | 65.0  |
| 0                             | 0   | 0     | 14                       | 70.0  |
| 0                             | 0   | 0     | 15                       | 75.0  |
| 1                             | 0   | 1     | 16                       | 80.0  |
| 0                             | 1   | 1     | 17                       | 85.0  |
| 1                             | 0   | 1     | 18                       | 90.0  |
| 0                             | 1   | 1     | 19                       | 95.0  |
| 5                             | 1   | 6     | 20                       | 100.0 |

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

### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ

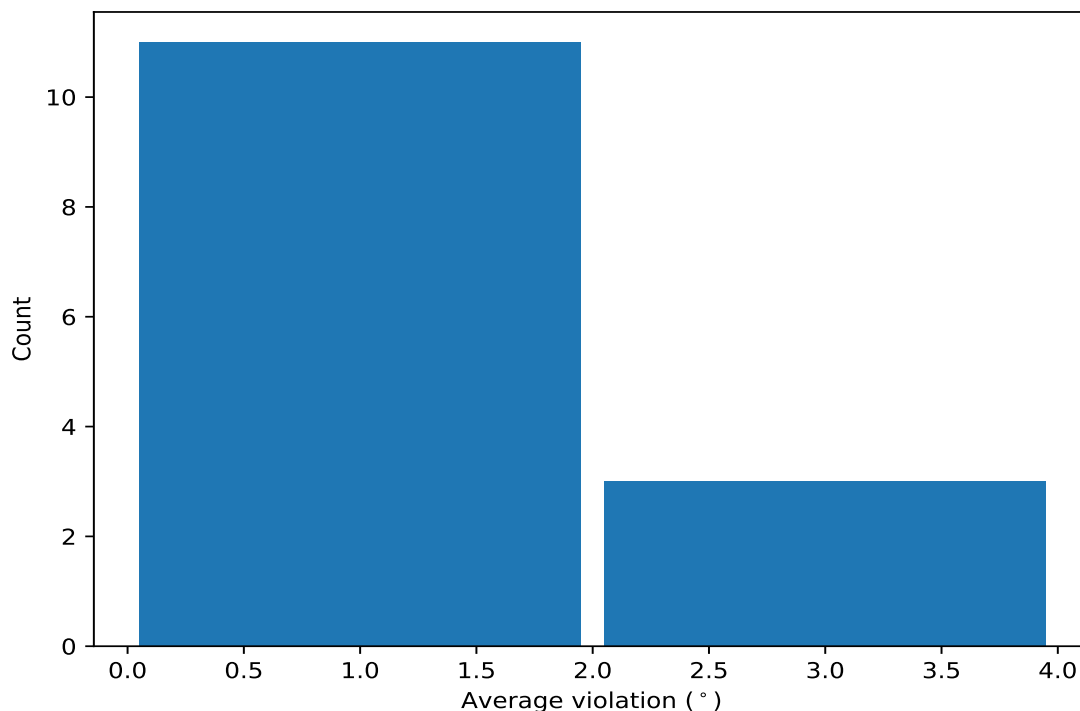


## 10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

### 10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



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

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

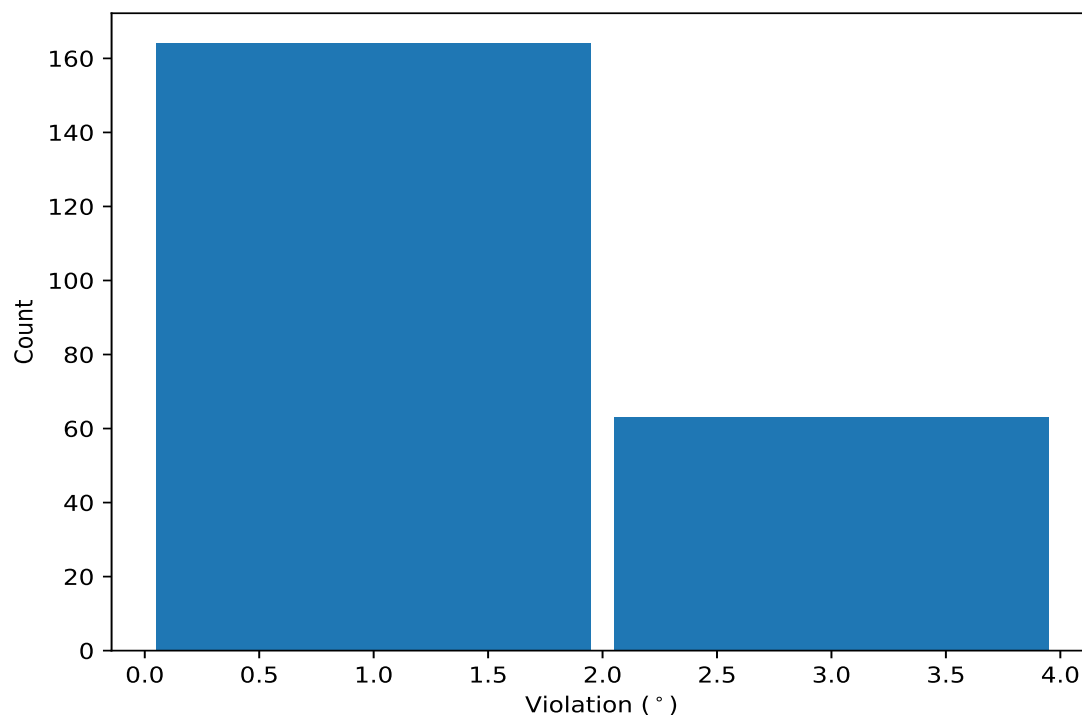
| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,9)   | 1:9:A:ARG:C  | 1:10:A:THR:N  | 1:10:A:THR:CA | 1:10:A:THR:C | 20                  | 3.22 | 0.23            | 3.18   |
| (1,80)  | 1:9:A:ARG:N  | 1:9:A:ARG:CA  | 1:9:A:ARG:C   | 1:10:A:THR:N | 20                  | 3.05 | 0.25            | 2.96   |
| (1,142) | 1:90:A:ALA:N | 1:90:A:ALA:CA | 1:90:A:ALA:C  | 1:91:A:TRP:N | 20                  | 2.29 | 0.08            | 2.27   |
| (1,81)  | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C  | 1:11:A:GLU:N | 20                  | 1.91 | 0.18            | 1.88   |
| (1,140) | 1:88:A:GLU:N | 1:88:A:GLU:CA | 1:88:A:GLU:C  | 1:89:A:ILE:N | 20                  | 1.74 | 0.09            | 1.78   |
| (1,121) | 1:65:A:ASP:N | 1:65:A:ASP:CA | 1:65:A:ASP:C  | 1:66:A:SER:N | 20                  | 1.39 | 0.09            | 1.39   |
| (1,7)   | 1:7:A:HIS:C  | 1:8:A:VAL:N   | 1:8:A:VAL:CA  | 1:8:A:VAL:C  | 19                  | 1.21 | 0.14            | 1.22   |
| (1,117) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C  | 1:61:A:SER:N | 18                  | 1.21 | 0.16            | 1.16   |
| (1,29)  | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 17                  | 1.24 | 0.17            | 1.27   |
| (1,114) | 1:57:A:MET:N | 1:57:A:MET:CA | 1:57:A:MET:C  | 1:58:A:ILE:N | 16                  | 1.18 | 0.13            | 1.14   |
| (1,139) | 1:86:A:SER:N | 1:86:A:SER:CA | 1:86:A:SER:C  | 1:87:A:LEU:N | 13                  | 1.32 | 0.15            | 1.28   |
| (1,51)  | 1:66:A:SER:C | 1:67:A:LEU:N  | 1:67:A:LEU:CA | 1:67:A:LEU:C | 9                   | 1.11 | 0.12            | 1.09   |
| (1,20)  | 1:22:A:LYS:C | 1:23:A:HIS:N  | 1:23:A:HIS:CA | 1:23:A:HIS:C | 9                   | 1.11 | 0.16            | 1.06   |
| (1,4)   | 1:4:A:SER:C  | 1:5:A:THR:N   | 1:5:A:THR:CA  | 1:5:A:THR:C  | 4                   | 1.04 | 0.03            | 1.03   |

<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 (°) |
|--------|-------------|--------------|---------------|--------------|----------|---------------|
| (1,9)  | 1:9:A:ARG:C | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C | 13       | 3.87          |
| (1,80) | 1:9:A:ARG:N | 1:9:A:ARG:CA | 1:9:A:ARG:C   | 1:10:A:THR:N | 13       | 3.76          |
| (1,9)  | 1:9:A:ARG:C | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C | 10       | 3.67          |
| (1,80) | 1:9:A:ARG:N | 1:9:A:ARG:CA | 1:9:A:ARG:C   | 1:10:A:THR:N | 10       | 3.5           |
| (1,9)  | 1:9:A:ARG:C | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C | 7        | 3.4           |
| (1,9)  | 1:9:A:ARG:C | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C | 17       | 3.39          |
| (1,80) | 1:9:A:ARG:N | 1:9:A:ARG:CA | 1:9:A:ARG:C   | 1:10:A:THR:N | 20       | 3.37          |
| (1,9)  | 1:9:A:ARG:C | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C | 2        | 3.29          |
| (1,9)  | 1:9:A:ARG:C | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C | 20       | 3.29          |
| (1,9)  | 1:9:A:ARG:C | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C | 6        | 3.28          |
| (1,9)  | 1:9:A:ARG:C | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C | 16       | 3.28          |
| (1,80) | 1:9:A:ARG:N | 1:9:A:ARG:CA | 1:9:A:ARG:C   | 1:10:A:THR:N | 17       | 3.27          |
| (1,9)  | 1:9:A:ARG:C | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C | 8        | 3.25          |
| (1,9)  | 1:9:A:ARG:C | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C | 4        | 3.19          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,9)   | 1:9:A:ARG:C  | 1:10:A:THR:N  | 1:10:A:THR:CA | 1:10:A:THR:C | 19       | 3.18          |
| (1,9)   | 1:9:A:ARG:C  | 1:10:A:THR:N  | 1:10:A:THR:CA | 1:10:A:THR:C | 12       | 3.15          |
| (1,80)  | 1:9:A:ARG:N  | 1:9:A:ARG:CA  | 1:9:A:ARG:C   | 1:10:A:THR:N | 7        | 3.13          |
| (1,80)  | 1:9:A:ARG:N  | 1:9:A:ARG:CA  | 1:9:A:ARG:C   | 1:10:A:THR:N | 2        | 3.12          |
| (1,80)  | 1:9:A:ARG:N  | 1:9:A:ARG:CA  | 1:9:A:ARG:C   | 1:10:A:THR:N | 6        | 3.12          |
| (1,9)   | 1:9:A:ARG:C  | 1:10:A:THR:N  | 1:10:A:THR:CA | 1:10:A:THR:C | 1        | 3.12          |
| (1,80)  | 1:9:A:ARG:N  | 1:9:A:ARG:CA  | 1:9:A:ARG:C   | 1:10:A:THR:N | 1        | 3.1           |
| (1,9)   | 1:9:A:ARG:C  | 1:10:A:THR:N  | 1:10:A:THR:CA | 1:10:A:THR:C | 18       | 3.1           |
| (1,9)   | 1:9:A:ARG:C  | 1:10:A:THR:N  | 1:10:A:THR:CA | 1:10:A:THR:C | 9        | 3.09          |
| (1,9)   | 1:9:A:ARG:C  | 1:10:A:THR:N  | 1:10:A:THR:CA | 1:10:A:THR:C | 15       | 3.07          |
| (1,9)   | 1:9:A:ARG:C  | 1:10:A:THR:N  | 1:10:A:THR:CA | 1:10:A:THR:C | 3        | 3.02          |
| (1,80)  | 1:9:A:ARG:N  | 1:9:A:ARG:CA  | 1:9:A:ARG:C   | 1:10:A:THR:N | 4        | 2.97          |
| (1,80)  | 1:9:A:ARG:N  | 1:9:A:ARG:CA  | 1:9:A:ARG:C   | 1:10:A:THR:N | 9        | 2.97          |
| (1,9)   | 1:9:A:ARG:C  | 1:10:A:THR:N  | 1:10:A:THR:CA | 1:10:A:THR:C | 11       | 2.97          |
| (1,80)  | 1:9:A:ARG:N  | 1:9:A:ARG:CA  | 1:9:A:ARG:C   | 1:10:A:THR:N | 19       | 2.96          |
| (1,9)   | 1:9:A:ARG:C  | 1:10:A:THR:N  | 1:10:A:THR:CA | 1:10:A:THR:C | 14       | 2.96          |
| (1,80)  | 1:9:A:ARG:N  | 1:9:A:ARG:CA  | 1:9:A:ARG:C   | 1:10:A:THR:N | 8        | 2.94          |
| (1,80)  | 1:9:A:ARG:N  | 1:9:A:ARG:CA  | 1:9:A:ARG:C   | 1:10:A:THR:N | 3        | 2.92          |
| (1,80)  | 1:9:A:ARG:N  | 1:9:A:ARG:CA  | 1:9:A:ARG:C   | 1:10:A:THR:N | 15       | 2.92          |
| (1,80)  | 1:9:A:ARG:N  | 1:9:A:ARG:CA  | 1:9:A:ARG:C   | 1:10:A:THR:N | 12       | 2.91          |
| (1,9)   | 1:9:A:ARG:C  | 1:10:A:THR:N  | 1:10:A:THR:CA | 1:10:A:THR:C | 5        | 2.91          |
| (1,80)  | 1:9:A:ARG:N  | 1:9:A:ARG:CA  | 1:9:A:ARG:C   | 1:10:A:THR:N | 5        | 2.88          |
| (1,80)  | 1:9:A:ARG:N  | 1:9:A:ARG:CA  | 1:9:A:ARG:C   | 1:10:A:THR:N | 16       | 2.88          |
| (1,80)  | 1:9:A:ARG:N  | 1:9:A:ARG:CA  | 1:9:A:ARG:C   | 1:10:A:THR:N | 18       | 2.83          |
| (1,80)  | 1:9:A:ARG:N  | 1:9:A:ARG:CA  | 1:9:A:ARG:C   | 1:10:A:THR:N | 11       | 2.82          |
| (1,80)  | 1:9:A:ARG:N  | 1:9:A:ARG:CA  | 1:9:A:ARG:C   | 1:10:A:THR:N | 14       | 2.69          |
| (1,142) | 1:90:A:ALA:N | 1:90:A:ALA:CA | 1:90:A:ALA:C  | 1:91:A:TRP:N | 5        | 2.43          |
| (1,142) | 1:90:A:ALA:N | 1:90:A:ALA:CA | 1:90:A:ALA:C  | 1:91:A:TRP:N | 15       | 2.43          |
| (1,142) | 1:90:A:ALA:N | 1:90:A:ALA:CA | 1:90:A:ALA:C  | 1:91:A:TRP:N | 10       | 2.42          |
| (1,142) | 1:90:A:ALA:N | 1:90:A:ALA:CA | 1:90:A:ALA:C  | 1:91:A:TRP:N | 20       | 2.38          |
| (1,142) | 1:90:A:ALA:N | 1:90:A:ALA:CA | 1:90:A:ALA:C  | 1:91:A:TRP:N | 8        | 2.35          |
| (1,81)  | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C  | 1:11:A:GLU:N | 16       | 2.35          |
| (1,142) | 1:90:A:ALA:N | 1:90:A:ALA:CA | 1:90:A:ALA:C  | 1:91:A:TRP:N | 12       | 2.34          |
| (1,142) | 1:90:A:ALA:N | 1:90:A:ALA:CA | 1:90:A:ALA:C  | 1:91:A:TRP:N | 18       | 2.34          |
| (1,142) | 1:90:A:ALA:N | 1:90:A:ALA:CA | 1:90:A:ALA:C  | 1:91:A:TRP:N | 2        | 2.3           |
| (1,81)  | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C  | 1:11:A:GLU:N | 14       | 2.3           |
| (1,142) | 1:90:A:ALA:N | 1:90:A:ALA:CA | 1:90:A:ALA:C  | 1:91:A:TRP:N | 7        | 2.28          |
| (1,142) | 1:90:A:ALA:N | 1:90:A:ALA:CA | 1:90:A:ALA:C  | 1:91:A:TRP:N | 14       | 2.28          |
| (1,142) | 1:90:A:ALA:N | 1:90:A:ALA:CA | 1:90:A:ALA:C  | 1:91:A:TRP:N | 11       | 2.26          |
| (1,142) | 1:90:A:ALA:N | 1:90:A:ALA:CA | 1:90:A:ALA:C  | 1:91:A:TRP:N | 3        | 2.24          |
| (1,142) | 1:90:A:ALA:N | 1:90:A:ALA:CA | 1:90:A:ALA:C  | 1:91:A:TRP:N | 13       | 2.24          |
| (1,142) | 1:90:A:ALA:N | 1:90:A:ALA:CA | 1:90:A:ALA:C  | 1:91:A:TRP:N | 4        | 2.23          |
| (1,142) | 1:90:A:ALA:N | 1:90:A:ALA:CA | 1:90:A:ALA:C  | 1:91:A:TRP:N | 17       | 2.23          |
| (1,142) | 1:90:A:ALA:N | 1:90:A:ALA:CA | 1:90:A:ALA:C  | 1:91:A:TRP:N | 16       | 2.22          |
| (1,142) | 1:90:A:ALA:N | 1:90:A:ALA:CA | 1:90:A:ALA:C  | 1:91:A:TRP:N | 19       | 2.22          |
| (1,142) | 1:90:A:ALA:N | 1:90:A:ALA:CA | 1:90:A:ALA:C  | 1:91:A:TRP:N | 6        | 2.2           |
| (1,142) | 1:90:A:ALA:N | 1:90:A:ALA:CA | 1:90:A:ALA:C  | 1:91:A:TRP:N | 1        | 2.18          |
| (1,142) | 1:90:A:ALA:N | 1:90:A:ALA:CA | 1:90:A:ALA:C  | 1:91:A:TRP:N | 9        | 2.18          |
| (1,81)  | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C  | 1:11:A:GLU:N | 13       | 2.12          |
| (1,81)  | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C  | 1:11:A:GLU:N | 2        | 1.98          |
| (1,81)  | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C  | 1:11:A:GLU:N | 10       | 1.97          |

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Continued from previous page...

| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,81)  | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C  | 1:11:A:GLU:N | 8        | 1.94          |
| (1,81)  | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C  | 1:11:A:GLU:N | 12       | 1.94          |
| (1,81)  | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C  | 1:11:A:GLU:N | 7        | 1.93          |
| (1,81)  | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C  | 1:11:A:GLU:N | 5        | 1.9           |
| (1,81)  | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C  | 1:11:A:GLU:N | 17       | 1.9           |
| (1,81)  | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C  | 1:11:A:GLU:N | 6        | 1.87          |
| (1,140) | 1:88:A:GLU:N | 1:88:A:GLU:CA | 1:88:A:GLU:C  | 1:89:A:ILE:N | 4        | 1.84          |
| (1,140) | 1:88:A:GLU:N | 1:88:A:GLU:CA | 1:88:A:GLU:C  | 1:89:A:ILE:N | 7        | 1.84          |
| (1,140) | 1:88:A:GLU:N | 1:88:A:GLU:CA | 1:88:A:GLU:C  | 1:89:A:ILE:N | 8        | 1.84          |
| (1,140) | 1:88:A:GLU:N | 1:88:A:GLU:CA | 1:88:A:GLU:C  | 1:89:A:ILE:N | 9        | 1.84          |
| (1,140) | 1:88:A:GLU:N | 1:88:A:GLU:CA | 1:88:A:GLU:C  | 1:89:A:ILE:N | 3        | 1.83          |
| (1,81)  | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C  | 1:11:A:GLU:N | 4        | 1.83          |
| (1,140) | 1:88:A:GLU:N | 1:88:A:GLU:CA | 1:88:A:GLU:C  | 1:89:A:ILE:N | 1        | 1.82          |
| (1,81)  | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C  | 1:11:A:GLU:N | 3        | 1.82          |
| (1,81)  | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C  | 1:11:A:GLU:N | 11       | 1.82          |
| (1,81)  | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C  | 1:11:A:GLU:N | 18       | 1.82          |
| (1,140) | 1:88:A:GLU:N | 1:88:A:GLU:CA | 1:88:A:GLU:C  | 1:89:A:ILE:N | 12       | 1.81          |
| (1,140) | 1:88:A:GLU:N | 1:88:A:GLU:CA | 1:88:A:GLU:C  | 1:89:A:ILE:N | 10       | 1.79          |
| (1,140) | 1:88:A:GLU:N | 1:88:A:GLU:CA | 1:88:A:GLU:C  | 1:89:A:ILE:N | 16       | 1.79          |
| (1,140) | 1:88:A:GLU:N | 1:88:A:GLU:CA | 1:88:A:GLU:C  | 1:89:A:ILE:N | 2        | 1.78          |
| (1,140) | 1:88:A:GLU:N | 1:88:A:GLU:CA | 1:88:A:GLU:C  | 1:89:A:ILE:N | 11       | 1.78          |
| (1,140) | 1:88:A:GLU:N | 1:88:A:GLU:CA | 1:88:A:GLU:C  | 1:89:A:ILE:N | 14       | 1.76          |
| (1,81)  | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C  | 1:11:A:GLU:N | 1        | 1.76          |
| (1,81)  | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C  | 1:11:A:GLU:N | 19       | 1.75          |
| (1,140) | 1:88:A:GLU:N | 1:88:A:GLU:CA | 1:88:A:GLU:C  | 1:89:A:ILE:N | 18       | 1.74          |
| (1,81)  | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C  | 1:11:A:GLU:N | 9        | 1.73          |
| (1,81)  | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C  | 1:11:A:GLU:N | 15       | 1.73          |
| (1,140) | 1:88:A:GLU:N | 1:88:A:GLU:CA | 1:88:A:GLU:C  | 1:89:A:ILE:N | 19       | 1.71          |
| (1,117) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C  | 1:61:A:SER:N | 2        | 1.67          |
| (1,140) | 1:88:A:GLU:N | 1:88:A:GLU:CA | 1:88:A:GLU:C  | 1:89:A:ILE:N | 6        | 1.65          |
| (1,81)  | 1:10:A:THR:N | 1:10:A:THR:CA | 1:10:A:THR:C  | 1:11:A:GLU:N | 20       | 1.65          |
| (1,140) | 1:88:A:GLU:N | 1:88:A:GLU:CA | 1:88:A:GLU:C  | 1:89:A:ILE:N | 13       | 1.62          |
| (1,140) | 1:88:A:GLU:N | 1:88:A:GLU:CA | 1:88:A:GLU:C  | 1:89:A:ILE:N | 15       | 1.61          |
| (1,140) | 1:88:A:GLU:N | 1:88:A:GLU:CA | 1:88:A:GLU:C  | 1:89:A:ILE:N | 17       | 1.61          |
| (1,140) | 1:88:A:GLU:N | 1:88:A:GLU:CA | 1:88:A:GLU:C  | 1:89:A:ILE:N | 20       | 1.61          |
| (1,121) | 1:65:A:ASP:N | 1:65:A:ASP:CA | 1:65:A:ASP:C  | 1:66:A:SER:N | 16       | 1.61          |
| (1,139) | 1:86:A:SER:N | 1:86:A:SER:CA | 1:86:A:SER:C  | 1:87:A:LEU:N | 17       | 1.59          |
| (1,140) | 1:88:A:GLU:N | 1:88:A:GLU:CA | 1:88:A:GLU:C  | 1:89:A:ILE:N | 5        | 1.57          |
| (1,121) | 1:65:A:ASP:N | 1:65:A:ASP:CA | 1:65:A:ASP:C  | 1:66:A:SER:N | 2        | 1.57          |
| (1,121) | 1:65:A:ASP:N | 1:65:A:ASP:CA | 1:65:A:ASP:C  | 1:66:A:SER:N | 9        | 1.57          |
| (1,20)  | 1:22:A:LYS:C | 1:23:A:HIS:N  | 1:23:A:HIS:CA | 1:23:A:HIS:C | 17       | 1.54          |
| (1,139) | 1:86:A:SER:N | 1:86:A:SER:CA | 1:86:A:SER:C  | 1:87:A:LEU:N | 14       | 1.53          |
| (1,29)  | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 20       | 1.52          |
| (1,7)   | 1:7:A:HIS:C  | 1:8:A:VAL:N   | 1:8:A:VAL:CA  | 1:8:A:VAL:C  | 17       | 1.49          |
| (1,139) | 1:86:A:SER:N | 1:86:A:SER:CA | 1:86:A:SER:C  | 1:87:A:LEU:N | 19       | 1.47          |
| (1,29)  | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 1        | 1.47          |
| (1,139) | 1:86:A:SER:N | 1:86:A:SER:CA | 1:86:A:SER:C  | 1:87:A:LEU:N | 9        | 1.44          |
| (1,114) | 1:57:A:MET:N | 1:57:A:MET:CA | 1:57:A:MET:C  | 1:58:A:ILE:N | 18       | 1.44          |
| (1,121) | 1:65:A:ASP:N | 1:65:A:ASP:CA | 1:65:A:ASP:C  | 1:66:A:SER:N | 4        | 1.42          |
| (1,121) | 1:65:A:ASP:N | 1:65:A:ASP:CA | 1:65:A:ASP:C  | 1:66:A:SER:N | 15       | 1.42          |
| (1,121) | 1:65:A:ASP:N | 1:65:A:ASP:CA | 1:65:A:ASP:C  | 1:66:A:SER:N | 1        | 1.41          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,121) | 1:65:A:ASP:N | 1:65:A:ASP:CA | 1:65:A:ASP:C  | 1:66:A:SER:N | 12       | 1.41          |
| (1,117) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C  | 1:61:A:SER:N | 4        | 1.41          |
| (1,91)  | 1:22:A:LYS:N | 1:22:A:LYS:CA | 1:22:A:LYS:C  | 1:23:A:HIS:N | 16       | 1.41          |
| (1,121) | 1:65:A:ASP:N | 1:65:A:ASP:CA | 1:65:A:ASP:C  | 1:66:A:SER:N | 8        | 1.4           |
| (1,121) | 1:65:A:ASP:N | 1:65:A:ASP:CA | 1:65:A:ASP:C  | 1:66:A:SER:N | 13       | 1.4           |
| (1,29)  | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 5        | 1.4           |
| (1,121) | 1:65:A:ASP:N | 1:65:A:ASP:CA | 1:65:A:ASP:C  | 1:66:A:SER:N | 11       | 1.39          |
| (1,121) | 1:65:A:ASP:N | 1:65:A:ASP:CA | 1:65:A:ASP:C  | 1:66:A:SER:N | 17       | 1.39          |
| (1,121) | 1:65:A:ASP:N | 1:65:A:ASP:CA | 1:65:A:ASP:C  | 1:66:A:SER:N | 10       | 1.38          |
| (1,117) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C  | 1:61:A:SER:N | 9        | 1.38          |
| (1,51)  | 1:66:A:SER:C | 1:67:A:LEU:N  | 1:67:A:LEU:CA | 1:67:A:LEU:C | 18       | 1.38          |
| (1,139) | 1:86:A:SER:N | 1:86:A:SER:CA | 1:86:A:SER:C  | 1:87:A:LEU:N | 6        | 1.37          |
| (1,114) | 1:57:A:MET:N | 1:57:A:MET:CA | 1:57:A:MET:C  | 1:58:A:ILE:N | 11       | 1.37          |
| (1,29)  | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 3        | 1.37          |
| (1,7)   | 1:7:A:HIS:C  | 1:8:A:VAL:N   | 1:8:A:VAL:CA  | 1:8:A:VAL:C  | 2        | 1.37          |
| (1,7)   | 1:7:A:HIS:C  | 1:8:A:VAL:N   | 1:8:A:VAL:CA  | 1:8:A:VAL:C  | 4        | 1.37          |
| (1,29)  | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 4        | 1.36          |
| (1,7)   | 1:7:A:HIS:C  | 1:8:A:VAL:N   | 1:8:A:VAL:CA  | 1:8:A:VAL:C  | 20       | 1.36          |
| (1,121) | 1:65:A:ASP:N | 1:65:A:ASP:CA | 1:65:A:ASP:C  | 1:66:A:SER:N | 5        | 1.35          |
| (1,29)  | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 12       | 1.35          |
| (1,7)   | 1:7:A:HIS:C  | 1:8:A:VAL:N   | 1:8:A:VAL:CA  | 1:8:A:VAL:C  | 10       | 1.35          |
| (1,121) | 1:65:A:ASP:N | 1:65:A:ASP:CA | 1:65:A:ASP:C  | 1:66:A:SER:N | 6        | 1.34          |
| (1,139) | 1:86:A:SER:N | 1:86:A:SER:CA | 1:86:A:SER:C  | 1:87:A:LEU:N | 7        | 1.33          |
| (1,29)  | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 9        | 1.33          |
| (1,29)  | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 19       | 1.33          |
| (1,114) | 1:57:A:MET:N | 1:57:A:MET:CA | 1:57:A:MET:C  | 1:58:A:ILE:N | 3        | 1.32          |
| (1,7)   | 1:7:A:HIS:C  | 1:8:A:VAL:N   | 1:8:A:VAL:CA  | 1:8:A:VAL:C  | 16       | 1.32          |
| (1,121) | 1:65:A:ASP:N | 1:65:A:ASP:CA | 1:65:A:ASP:C  | 1:66:A:SER:N | 3        | 1.31          |
| (1,121) | 1:65:A:ASP:N | 1:65:A:ASP:CA | 1:65:A:ASP:C  | 1:66:A:SER:N | 19       | 1.31          |
| (1,121) | 1:65:A:ASP:N | 1:65:A:ASP:CA | 1:65:A:ASP:C  | 1:66:A:SER:N | 20       | 1.31          |
| (1,117) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C  | 1:61:A:SER:N | 5        | 1.31          |
| (1,121) | 1:65:A:ASP:N | 1:65:A:ASP:CA | 1:65:A:ASP:C  | 1:66:A:SER:N | 14       | 1.3           |
| (1,121) | 1:65:A:ASP:N | 1:65:A:ASP:CA | 1:65:A:ASP:C  | 1:66:A:SER:N | 18       | 1.3           |
| (1,117) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C  | 1:61:A:SER:N | 18       | 1.3           |
| (1,114) | 1:57:A:MET:N | 1:57:A:MET:CA | 1:57:A:MET:C  | 1:58:A:ILE:N | 8        | 1.3           |
| (1,114) | 1:57:A:MET:N | 1:57:A:MET:CA | 1:57:A:MET:C  | 1:58:A:ILE:N | 12       | 1.29          |
| (1,139) | 1:86:A:SER:N | 1:86:A:SER:CA | 1:86:A:SER:C  | 1:87:A:LEU:N | 16       | 1.28          |
| (1,121) | 1:65:A:ASP:N | 1:65:A:ASP:CA | 1:65:A:ASP:C  | 1:66:A:SER:N | 7        | 1.28          |
| (1,29)  | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 11       | 1.27          |
| (1,139) | 1:86:A:SER:N | 1:86:A:SER:CA | 1:86:A:SER:C  | 1:87:A:LEU:N | 1        | 1.26          |
| (1,117) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C  | 1:61:A:SER:N | 8        | 1.26          |
| (1,117) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C  | 1:61:A:SER:N | 11       | 1.26          |
| (1,114) | 1:57:A:MET:N | 1:57:A:MET:CA | 1:57:A:MET:C  | 1:58:A:ILE:N | 6        | 1.26          |
| (1,29)  | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 15       | 1.26          |
| (1,7)   | 1:7:A:HIS:C  | 1:8:A:VAL:N   | 1:8:A:VAL:CA  | 1:8:A:VAL:C  | 3        | 1.26          |
| (1,139) | 1:86:A:SER:N | 1:86:A:SER:CA | 1:86:A:SER:C  | 1:87:A:LEU:N | 3        | 1.25          |
| (1,51)  | 1:66:A:SER:C | 1:67:A:LEU:N  | 1:67:A:LEU:CA | 1:67:A:LEU:C | 6        | 1.25          |
| (1,139) | 1:86:A:SER:N | 1:86:A:SER:CA | 1:86:A:SER:C  | 1:87:A:LEU:N | 18       | 1.24          |
| (1,7)   | 1:7:A:HIS:C  | 1:8:A:VAL:N   | 1:8:A:VAL:CA  | 1:8:A:VAL:C  | 1        | 1.24          |
| (1,114) | 1:57:A:MET:N | 1:57:A:MET:CA | 1:57:A:MET:C  | 1:58:A:ILE:N | 14       | 1.23          |
| (1,7)   | 1:7:A:HIS:C  | 1:8:A:VAL:N   | 1:8:A:VAL:CA  | 1:8:A:VAL:C  | 6        | 1.23          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,117) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C  | 1:61:A:SER:N | 13       | 1.22          |
| (1,7)   | 1:7:A:HIS:C  | 1:8:A:VAL:N   | 1:8:A:VAL:CA  | 1:8:A:VAL:C  | 5        | 1.22          |
| (1,7)   | 1:7:A:HIS:C  | 1:8:A:VAL:N   | 1:8:A:VAL:CA  | 1:8:A:VAL:C  | 7        | 1.21          |
| (1,117) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C  | 1:61:A:SER:N | 15       | 1.19          |
| (1,29)  | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 8        | 1.17          |
| (1,139) | 1:86:A:SER:N | 1:86:A:SER:CA | 1:86:A:SER:C  | 1:87:A:LEU:N | 15       | 1.15          |
| (1,114) | 1:57:A:MET:N | 1:57:A:MET:CA | 1:57:A:MET:C  | 1:58:A:ILE:N | 10       | 1.15          |
| (1,114) | 1:57:A:MET:N | 1:57:A:MET:CA | 1:57:A:MET:C  | 1:58:A:ILE:N | 4        | 1.14          |
| (1,114) | 1:57:A:MET:N | 1:57:A:MET:CA | 1:57:A:MET:C  | 1:58:A:ILE:N | 15       | 1.14          |
| (1,139) | 1:86:A:SER:N | 1:86:A:SER:CA | 1:86:A:SER:C  | 1:87:A:LEU:N | 20       | 1.13          |
| (1,51)  | 1:66:A:SER:C | 1:67:A:LEU:N  | 1:67:A:LEU:CA | 1:67:A:LEU:C | 15       | 1.13          |
| (1,7)   | 1:7:A:HIS:C  | 1:8:A:VAL:N   | 1:8:A:VAL:CA  | 1:8:A:VAL:C  | 19       | 1.13          |
| (1,139) | 1:86:A:SER:N | 1:86:A:SER:CA | 1:86:A:SER:C  | 1:87:A:LEU:N | 12       | 1.12          |
| (1,117) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C  | 1:61:A:SER:N | 7        | 1.12          |
| (1,117) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C  | 1:61:A:SER:N | 17       | 1.12          |
| (1,20)  | 1:22:A:LYS:C | 1:23:A:HIS:N  | 1:23:A:HIS:CA | 1:23:A:HIS:C | 15       | 1.11          |
| (1,117) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C  | 1:61:A:SER:N | 1        | 1.1           |
| (1,117) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C  | 1:61:A:SER:N | 16       | 1.1           |
| (1,117) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C  | 1:61:A:SER:N | 19       | 1.1           |
| (1,7)   | 1:7:A:HIS:C  | 1:8:A:VAL:N   | 1:8:A:VAL:CA  | 1:8:A:VAL:C  | 14       | 1.1           |
| (1,51)  | 1:66:A:SER:C | 1:67:A:LEU:N  | 1:67:A:LEU:CA | 1:67:A:LEU:C | 5        | 1.09          |
| (1,51)  | 1:66:A:SER:C | 1:67:A:LEU:N  | 1:67:A:LEU:CA | 1:67:A:LEU:C | 13       | 1.09          |
| (1,20)  | 1:22:A:LYS:C | 1:23:A:HIS:N  | 1:23:A:HIS:CA | 1:23:A:HIS:C | 19       | 1.09          |
| (1,7)   | 1:7:A:HIS:C  | 1:8:A:VAL:N   | 1:8:A:VAL:CA  | 1:8:A:VAL:C  | 13       | 1.09          |
| (1,114) | 1:57:A:MET:N | 1:57:A:MET:CA | 1:57:A:MET:C  | 1:58:A:ILE:N | 2        | 1.08          |
| (1,29)  | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 6        | 1.08          |
| (1,20)  | 1:22:A:LYS:C | 1:23:A:HIS:N  | 1:23:A:HIS:CA | 1:23:A:HIS:C | 20       | 1.08          |
| (1,4)   | 1:4:A:SER:C  | 1:5:A:THR:N   | 1:5:A:THR:CA  | 1:5:A:THR:C  | 20       | 1.08          |
| (1,117) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C  | 1:61:A:SER:N | 10       | 1.07          |
| (1,114) | 1:57:A:MET:N | 1:57:A:MET:CA | 1:57:A:MET:C  | 1:58:A:ILE:N | 5        | 1.07          |
| (1,7)   | 1:7:A:HIS:C  | 1:8:A:VAL:N   | 1:8:A:VAL:CA  | 1:8:A:VAL:C  | 18       | 1.07          |
| (1,117) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C  | 1:61:A:SER:N | 3        | 1.06          |
| (1,29)  | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 14       | 1.06          |
| (1,20)  | 1:22:A:LYS:C | 1:23:A:HIS:N  | 1:23:A:HIS:CA | 1:23:A:HIS:C | 1        | 1.06          |
| (1,20)  | 1:22:A:LYS:C | 1:23:A:HIS:N  | 1:23:A:HIS:CA | 1:23:A:HIS:C | 10       | 1.06          |
| (1,126) | 1:70:A:MET:N | 1:70:A:MET:CA | 1:70:A:MET:C  | 1:71:A:GLN:N | 19       | 1.05          |
| (1,29)  | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 17       | 1.05          |
| (1,117) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C  | 1:61:A:SER:N | 6        | 1.04          |
| (1,117) | 1:60:A:ASN:N | 1:60:A:ASN:CA | 1:60:A:ASN:C  | 1:61:A:SER:N | 20       | 1.04          |
| (1,114) | 1:57:A:MET:N | 1:57:A:MET:CA | 1:57:A:MET:C  | 1:58:A:ILE:N | 13       | 1.04          |
| (1,7)   | 1:7:A:HIS:C  | 1:8:A:VAL:N   | 1:8:A:VAL:CA  | 1:8:A:VAL:C  | 12       | 1.04          |
| (1,7)   | 1:7:A:HIS:C  | 1:8:A:VAL:N   | 1:8:A:VAL:CA  | 1:8:A:VAL:C  | 15       | 1.04          |
| (1,4)   | 1:4:A:SER:C  | 1:5:A:THR:N   | 1:5:A:THR:CA  | 1:5:A:THR:C  | 13       | 1.04          |
| (1,114) | 1:57:A:MET:N | 1:57:A:MET:CA | 1:57:A:MET:C  | 1:58:A:ILE:N | 17       | 1.03          |
| (1,20)  | 1:22:A:LYS:C | 1:23:A:HIS:N  | 1:23:A:HIS:CA | 1:23:A:HIS:C | 4        | 1.03          |
| (1,7)   | 1:7:A:HIS:C  | 1:8:A:VAL:N   | 1:8:A:VAL:CA  | 1:8:A:VAL:C  | 11       | 1.03          |
| (1,114) | 1:57:A:MET:N | 1:57:A:MET:CA | 1:57:A:MET:C  | 1:58:A:ILE:N | 9        | 1.02          |
| (1,51)  | 1:66:A:SER:C | 1:67:A:LEU:N  | 1:67:A:LEU:CA | 1:67:A:LEU:C | 3        | 1.02          |
| (1,51)  | 1:66:A:SER:C | 1:67:A:LEU:N  | 1:67:A:LEU:CA | 1:67:A:LEU:C | 16       | 1.02          |
| (1,29)  | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 2        | 1.02          |
| (1,29)  | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 13       | 1.02          |

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*Continued from previous page...*

| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,4)   | 1:4:A:SER:C  | 1:5:A:THR:N   | 1:5:A:THR:CA  | 1:5:A:THR:C  | 18       | 1.02          |
| (1,114) | 1:57:A:MET:N | 1:57:A:MET:CA | 1:57:A:MET:C  | 1:58:A:ILE:N | 7        | 1.01          |
| (1,51)  | 1:66:A:SER:C | 1:67:A:LEU:N  | 1:67:A:LEU:CA | 1:67:A:LEU:C | 8        | 1.01          |
| (1,29)  | 1:35:A:GLU:C | 1:36:A:ARG:N  | 1:36:A:ARG:CA | 1:36:A:ARG:C | 16       | 1.01          |
| (1,4)   | 1:4:A:SER:C  | 1:5:A:THR:N   | 1:5:A:THR:CA  | 1:5:A:THR:C  | 10       | 1.01          |
| (1,51)  | 1:66:A:SER:C | 1:67:A:LEU:N  | 1:67:A:LEU:CA | 1:67:A:LEU:C | 11       | 1.0           |
| (1,20)  | 1:22:A:LYS:C | 1:23:A:HIS:N  | 1:23:A:HIS:CA | 1:23:A:HIS:C | 12       | 1.0           |
| (1,20)  | 1:22:A:LYS:C | 1:23:A:HIS:N  | 1:23:A:HIS:CA | 1:23:A:HIS:C | 14       | 1.0           |
| (1,7)   | 1:7:A:HIS:C  | 1:8:A:VAL:N   | 1:8:A:VAL:CA  | 1:8:A:VAL:C  | 8        | 1.0           |