



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 08:10 PM UTC

PDB ID : 2NSW / pdb\_00002nsw  
BMRB ID : 7327  
Title : NMR Solution Structure of the Pheromone En-2  
Authors : Placzek, W.J.; Etezady-Esfarjani, T.; Herrmann, T.; Peti, W.; Wuthrich, K.  
Deposited on : 2006-11-06

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

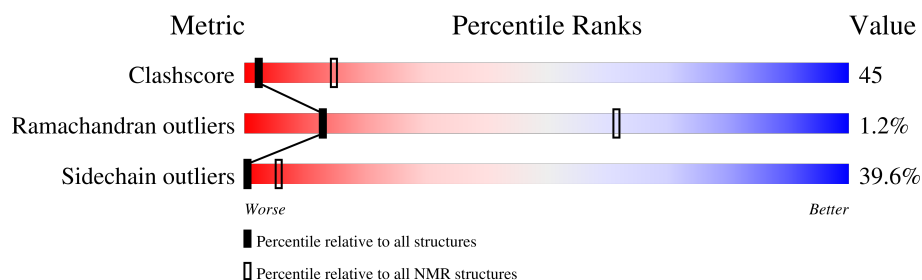
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 60%.

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     | 60     | <div> <div></div> <div>22%</div> <div>43%</div> <div>15%</div> <div>20%</div> </div> |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

| Well-defined (core) protein residues |                          |                   |              |
|--------------------------------------|--------------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total)    | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:2-A:26, A:30-A:52 (48) | 0.27              | 3            |

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

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

The models can be grouped into 4 clusters. No single-model clusters were found.

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

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

There is only 1 type of molecule in this entry. The entry contains 795 atoms, of which 362 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Mating pheromone En-2.

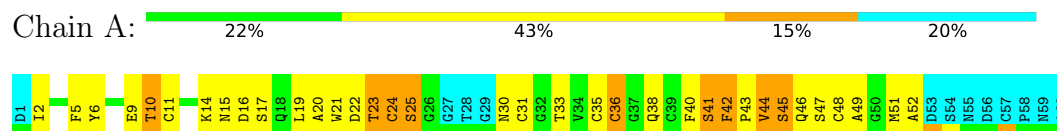
| Mol | Chain | Residues | Atoms |     |     |    |    |   | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|-------|
| 1   | A     | 60       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 795   | 258 | 362 | 69 | 97 | 9 |       |

## 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: Mating pheromone En-2

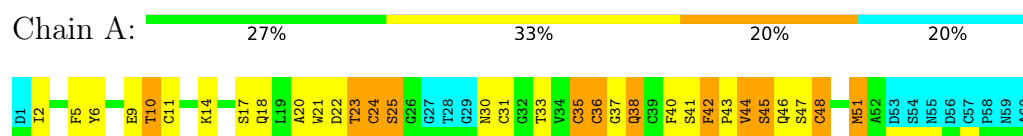


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

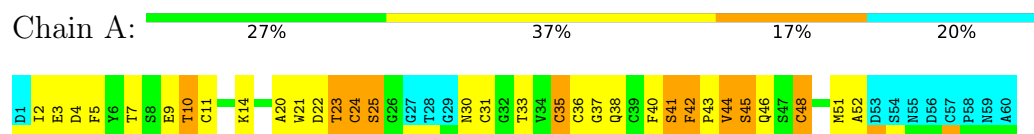
#### 4.2.1 Score per residue for model 1

- Molecule 1: Mating pheromone En-2



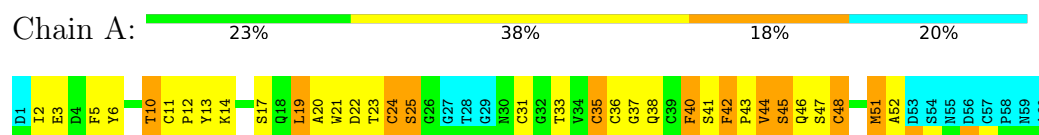
#### 4.2.2 Score per residue for model 2

- Molecule 1: Mating pheromone En-2



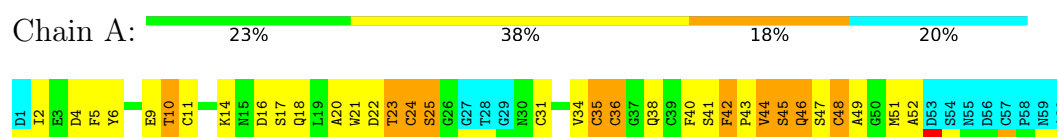
### 4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Mating pheromone En-2



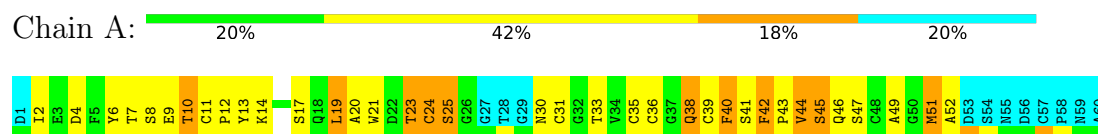
### 4.2.4 Score per residue for model 4

- Molecule 1: Mating pheromone En-2



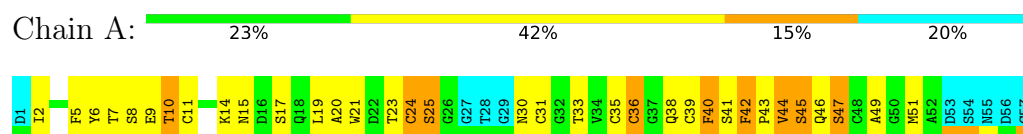
### 4.2.5 Score per residue for model 5

- Molecule 1: Mating pheromone En-2



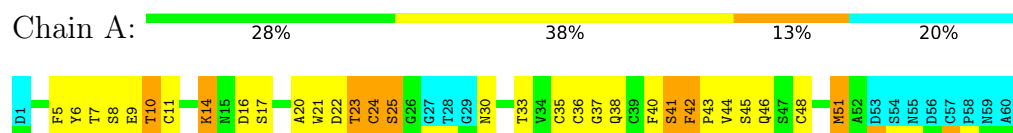
### 4.2.6 Score per residue for model 6

- Molecule 1: Mating pheromone En-2



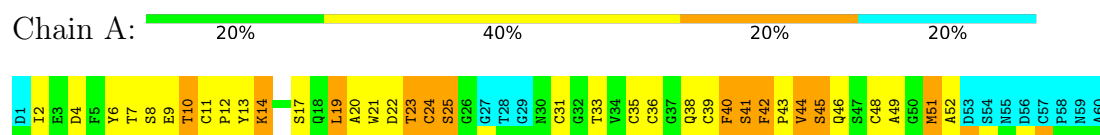
### 4.2.7 Score per residue for model 7

- Molecule 1: Mating pheromone En-2



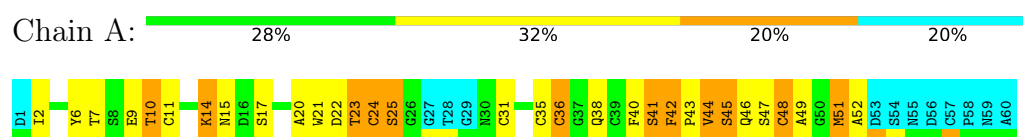
### 4.2.8 Score per residue for model 8

- Molecule 1: Mating pheromone En-2



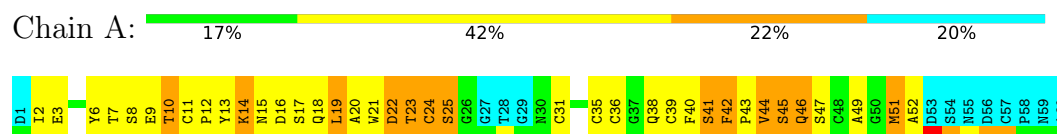
### 4.2.9 Score per residue for model 9

- Molecule 1: Mating pheromone En-2



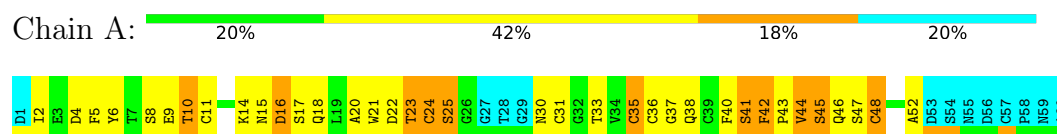
### 4.2.10 Score per residue for model 10

- Molecule 1: Mating pheromone En-2



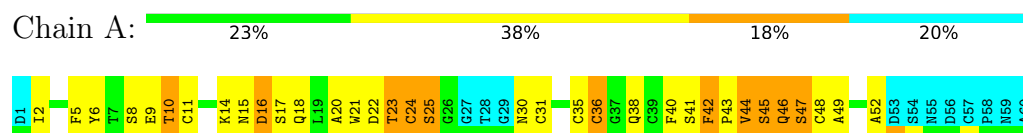
### 4.2.11 Score per residue for model 11

- Molecule 1: Mating pheromone En-2



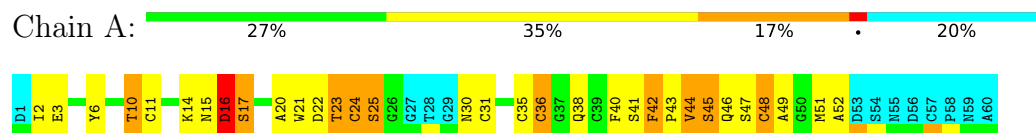
### 4.2.12 Score per residue for model 12

- Molecule 1: Mating pheromone En-2



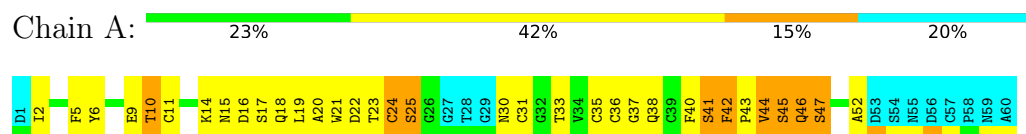
### 4.2.13 Score per residue for model 13

- Molecule 1: Mating pheromone En-2



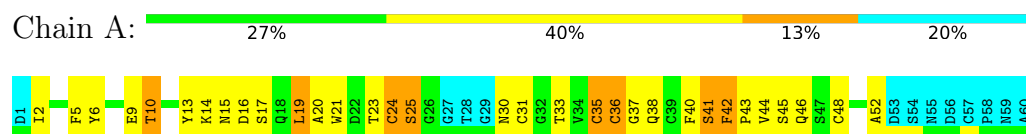
### 4.2.14 Score per residue for model 14

- Molecule 1: Mating pheromone En-2



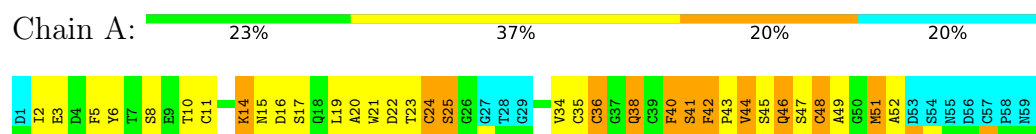
### 4.2.15 Score per residue for model 15

- Molecule 1: Mating pheromone En-2



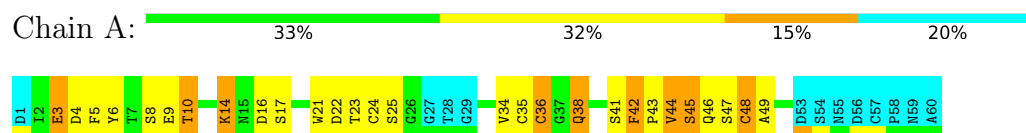
### 4.2.16 Score per residue for model 16

- Molecule 1: Mating pheromone En-2



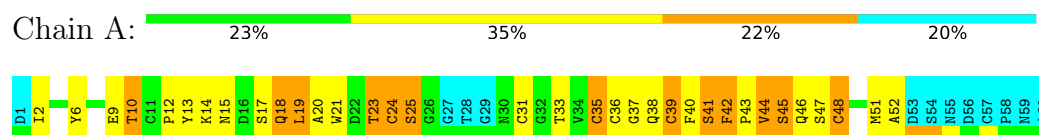
### 4.2.17 Score per residue for model 17

- Molecule 1: Mating pheromone En-2



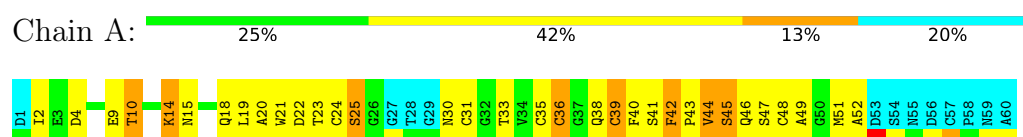
### 4.2.18 Score per residue for model 18

- Molecule 1: Mating pheromone En-2



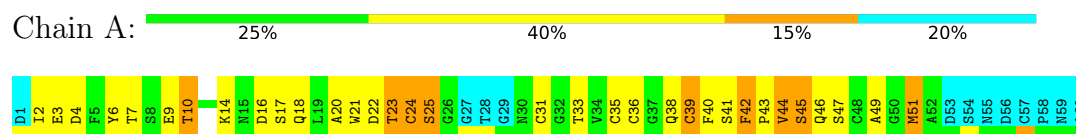
### 4.2.19 Score per residue for model 19

- Molecule 1: Mating pheromone En-2



### 4.2.20 Score per residue for model 20

- Molecule 1: Mating pheromone En-2



## 5 Refinement protocol and experimental data overview

Of the 80 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

| Software name | Classification | Version |
|---------------|----------------|---------|
| DYANA         | refinement     |         |

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

|                                              |                |
|----------------------------------------------|----------------|
| Chemical shift file(s)                       | working_cs.cif |
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 389            |
| Number of shifts mapped to atoms             | 389            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 60%            |

## 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     | 354   | 304      | 305      | 29±3    |
| All | All   | 7080  | 6080     | 6100     | 587     |

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 45.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:10:THR:HG23 | 1:A:38:GLN:O    | 0.88     | 1.69        | 18     | 20    |
| 1:A:19:LEU:HD13 | 1:A:20:ALA:N    | 0.82     | 1.89        | 18     | 6     |
| 1:A:36:CYS:SG   | 1:A:49:ALA:HB2  | 0.74     | 2.23        | 17     | 12    |
| 1:A:15:ASN:HB3  | 1:A:19:LEU:HD22 | 0.71     | 1.61        | 6      | 2     |
| 1:A:19:LEU:HD13 | 1:A:19:LEU:C    | 0.69     | 2.13        | 18     | 6     |
| 1:A:15:ASN:CB   | 1:A:19:LEU:HD22 | 0.67     | 2.19        | 6      | 2     |
| 1:A:5:PHE:CG    | 1:A:44:VAL:HG21 | 0.66     | 2.25        | 1      | 12    |
| 1:A:42:PHE:CD2  | 1:A:43:PRO:HA   | 0.64     | 2.27        | 11     | 20    |
| 1:A:23:THR:HG22 | 1:A:24:CYS:N    | 0.62     | 2.10        | 10     | 7     |
| 1:A:42:PHE:CG   | 1:A:43:PRO:HA   | 0.60     | 2.31        | 3      | 20    |
| 1:A:21:TRP:CE3  | 1:A:25:SER:OG   | 0.60     | 2.54        | 19     | 9     |
| 1:A:21:TRP:CZ2  | 1:A:51:MET:CB   | 0.59     | 2.86        | 10     | 11    |
| 1:A:21:TRP:CG   | 1:A:25:SER:HG   | 0.58     | 2.17        | 6      | 6     |
| 1:A:6:TYR:CG    | 1:A:17:SER:CB   | 0.56     | 2.89        | 13     | 1     |

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| Atom-1         | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|----------------|-----------------|----------|-------------|--------|-------|
|                |                 |          |             | Worst  | Total |
| 1:A:48:CYS:O   | 1:A:52:ALA:HB2  | 0.56     | 2.01        | 11     | 5     |
| 1:A:20:ALA:CB  | 1:A:39:CYS:SG   | 0.56     | 2.94        | 19     | 3     |
| 1:A:15:ASN:O   | 1:A:16:ASP:CB   | 0.56     | 2.54        | 14     | 4     |
| 1:A:6:TYR:CG   | 1:A:17:SER:OG   | 0.55     | 2.58        | 13     | 1     |
| 1:A:36:CYS:SG  | 1:A:37:GLY:N    | 0.55     | 2.79        | 7      | 8     |
| 1:A:34:VAL:CG1 | 1:A:38:GLN:NE2  | 0.55     | 2.70        | 16     | 1     |
| 1:A:19:LEU:CD1 | 1:A:20:ALA:N    | 0.55     | 2.69        | 18     | 1     |
| 1:A:21:TRP:CD2 | 1:A:25:SER:OG   | 0.54     | 2.59        | 3      | 9     |
| 1:A:24:CYS:SG  | 1:A:25:SER:N    | 0.53     | 2.80        | 14     | 12    |
| 1:A:5:PHE:CB   | 1:A:44:VAL:HG21 | 0.53     | 2.33        | 1      | 2     |
| 1:A:42:PHE:CE1 | 1:A:46:GLN:HB2  | 0.52     | 2.40        | 8      | 20    |
| 1:A:13:TYR:CD1 | 1:A:19:LEU:HD11 | 0.52     | 2.40        | 3      | 4     |
| 1:A:15:ASN:HB2 | 1:A:19:LEU:HD22 | 0.52     | 1.82        | 14     | 1     |
| 1:A:18:GLN:O   | 1:A:22:ASP:CB   | 0.52     | 2.58        | 14     | 3     |
| 1:A:39:CYS:HB3 | 1:A:40:PHE:CE1  | 0.51     | 2.40        | 19     | 3     |
| 1:A:24:CYS:O   | 1:A:31:CYS:CB   | 0.51     | 2.59        | 3      | 11    |
| 1:A:21:TRP:CZ2 | 1:A:51:MET:HB3  | 0.51     | 2.41        | 9      | 7     |
| 1:A:11:CYS:SG  | 1:A:20:ALA:CB   | 0.50     | 2.99        | 8      | 15    |
| 1:A:21:TRP:HB2 | 1:A:40:PHE:CZ   | 0.50     | 2.42        | 15     | 17    |
| 1:A:42:PHE:HA  | 1:A:43:PRO:C    | 0.50     | 2.32        | 17     | 20    |
| 1:A:41:SER:O   | 1:A:44:VAL:HB   | 0.49     | 2.07        | 15     | 20    |
| 1:A:42:PHE:CZ  | 1:A:46:GLN:HB2  | 0.49     | 2.43        | 8      | 11    |
| 1:A:10:THR:CG2 | 1:A:38:GLN:O    | 0.49     | 2.57        | 10     | 13    |
| 1:A:21:TRP:CE2 | 1:A:25:SER:OG   | 0.48     | 2.56        | 17     | 1     |
| 1:A:23:THR:CG2 | 1:A:24:CYS:N    | 0.48     | 2.77        | 10     | 3     |
| 1:A:13:TYR:HB3 | 1:A:19:LEU:HD12 | 0.47     | 1.84        | 15     | 4     |
| 1:A:19:LEU:C   | 1:A:19:LEU:CD1  | 0.47     | 2.86        | 18     | 1     |
| 1:A:6:TYR:CG   | 1:A:17:SER:HB3  | 0.47     | 2.45        | 9      | 13    |
| 1:A:41:SER:O   | 1:A:44:VAL:CB   | 0.47     | 2.63        | 15     | 19    |
| 1:A:23:THR:CG2 | 1:A:30:ASN:OD1  | 0.47     | 2.63        | 12     | 2     |
| 1:A:40:PHE:CD1 | 1:A:40:PHE:N    | 0.47     | 2.83        | 6      | 1     |
| 1:A:6:TYR:CG   | 1:A:17:SER:HB2  | 0.47     | 2.45        | 17     | 4     |
| 1:A:7:THR:N    | 1:A:39:CYS:O    | 0.47     | 2.48        | 8      | 3     |
| 1:A:21:TRP:CD1 | 1:A:25:SER:HG   | 0.46     | 2.28        | 17     | 1     |
| 1:A:21:TRP:CE2 | 1:A:25:SER:HB2  | 0.46     | 2.46        | 18     | 15    |
| 1:A:21:TRP:CD1 | 1:A:25:SER:OG   | 0.46     | 2.68        | 17     | 1     |
| 1:A:35:CYS:C   | 1:A:48:CYS:SG   | 0.46     | 2.99        | 3      | 7     |
| 1:A:42:PHE:N   | 1:A:45:SER:HB3  | 0.46     | 2.26        | 6      | 15    |
| 1:A:36:CYS:SG  | 1:A:45:SER:O    | 0.46     | 2.73        | 20     | 12    |
| 1:A:30:ASN:OD1 | 1:A:30:ASN:C    | 0.46     | 2.59        | 13     | 3     |
| 1:A:42:PHE:HA  | 1:A:44:VAL:N    | 0.46     | 2.25        | 15     | 18    |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:44:VAL:C    | 1:A:46:GLN:N    | 0.45     | 2.74        | 20     | 18    |
| 1:A:12:PRO:HG2  | 1:A:13:TYR:CE2  | 0.45     | 2.46        | 8      | 5     |
| 1:A:7:THR:OG1   | 1:A:10:THR:CG2  | 0.45     | 2.64        | 7      | 2     |
| 1:A:21:TRP:O    | 1:A:25:SER:N    | 0.45     | 2.49        | 6      | 1     |
| 1:A:21:TRP:CZ2  | 1:A:51:MET:SD   | 0.45     | 3.09        | 1      | 1     |
| 1:A:44:VAL:O    | 1:A:47:SER:N    | 0.45     | 2.49        | 16     | 14    |
| 1:A:36:CYS:N    | 1:A:48:CYS:SG   | 0.45     | 2.89        | 15     | 8     |
| 1:A:21:TRP:CD2  | 1:A:25:SER:CB   | 0.45     | 2.99        | 19     | 1     |
| 1:A:31:CYS:HB2  | 1:A:52:ALA:HB1  | 0.45     | 1.89        | 14     | 1     |
| 1:A:21:TRP:CG   | 1:A:25:SER:OG   | 0.44     | 2.70        | 17     | 1     |
| 1:A:36:CYS:O    | 1:A:40:PHE:O    | 0.44     | 2.36        | 10     | 16    |
| 1:A:14:LYS:O    | 1:A:15:ASN:CB   | 0.44     | 2.66        | 9      | 2     |
| 1:A:5:PHE:CG    | 1:A:44:VAL:CG2  | 0.44     | 2.99        | 1      | 2     |
| 1:A:18:GLN:O    | 1:A:22:ASP:N    | 0.44     | 2.50        | 19     | 6     |
| 1:A:36:CYS:SG   | 1:A:49:ALA:CB   | 0.44     | 3.03        | 17     | 2     |
| 1:A:25:SER:O    | 1:A:51:MET:SD   | 0.43     | 2.77        | 1      | 1     |
| 1:A:33:THR:O    | 1:A:36:CYS:SG   | 0.43     | 2.77        | 19     | 12    |
| 1:A:41:SER:C    | 1:A:45:SER:H    | 0.43     | 2.22        | 4      | 9     |
| 1:A:21:TRP:O    | 1:A:25:SER:OG   | 0.43     | 2.36        | 17     | 1     |
| 1:A:14:LYS:N    | 1:A:14:LYS:CD   | 0.43     | 2.82        | 17     | 2     |
| 1:A:22:ASP:O    | 1:A:22:ASP:OD1  | 0.43     | 2.37        | 17     | 1     |
| 1:A:6:TYR:CD2   | 1:A:17:SER:HB3  | 0.43     | 2.48        | 12     | 2     |
| 1:A:20:ALA:HB1  | 1:A:39:CYS:SG   | 0.43     | 2.53        | 20     | 3     |
| 1:A:18:GLN:O    | 1:A:22:ASP:CG   | 0.43     | 2.62        | 11     | 1     |
| 1:A:7:THR:OG1   | 1:A:7:THR:O     | 0.42     | 2.36        | 7      | 1     |
| 1:A:19:LEU:HD13 | 1:A:20:ALA:CA   | 0.42     | 2.45        | 18     | 1     |
| 1:A:18:GLN:NE2  | 1:A:18:GLN:O    | 0.42     | 2.53        | 18     | 1     |
| 1:A:7:THR:O     | 1:A:7:THR:OG1   | 0.42     | 2.37        | 2      | 5     |
| 1:A:33:THR:HA   | 1:A:36:CYS:SG   | 0.41     | 2.55        | 20     | 1     |
| 1:A:30:ASN:O    | 1:A:30:ASN:CG   | 0.41     | 2.62        | 5      | 1     |
| 1:A:21:TRP:NE1  | 1:A:25:SER:HG   | 0.41     | 2.07        | 17     | 1     |
| 1:A:31:CYS:SG   | 1:A:52:ALA:O    | 0.41     | 2.79        | 13     | 8     |
| 1:A:13:TYR:CG   | 1:A:19:LEU:CD1  | 0.41     | 3.03        | 10     | 1     |
| 1:A:14:LYS:HD3  | 1:A:14:LYS:N    | 0.41     | 2.31        | 19     | 2     |
| 1:A:14:LYS:N    | 1:A:14:LYS:HD3  | 0.41     | 2.31        | 10     | 1     |
| 1:A:34:VAL:HG12 | 1:A:38:GLN:NE2  | 0.40     | 2.32        | 4      | 1     |
| 1:A:41:SER:O    | 1:A:44:VAL:HG23 | 0.40     | 2.17        | 15     | 1     |
| 1:A:34:VAL:O    | 1:A:38:GLN:HB2  | 0.40     | 2.17        | 17     | 1     |
| 1:A:14:LYS:O    | 1:A:19:LEU:HD23 | 0.40     | 2.17        | 16     | 1     |

## 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed       | Favoured      | Allowed     | Outliers   | Percentiles |    |
|-----|-------|----------------|---------------|-------------|------------|-------------|----|
| 1   | A     | 48/60 (80%)    | 38±8 (78±17%) | 7±2 (14±4%) | 1±1 (1±1%) | 14          | 63 |
| All | All   | 899/1200 (75%) | 750 (83%)     | 138 (15%)   | 11 (1%)    | 13          | 61 |

All 2 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     | 36  | CYS  | 8              |
| 1   | A     | 16  | ASP  | 3              |

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

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

| Mol | Chain | Analysed       | Rotameric    | Outliers     | Percentiles |   |
|-----|-------|----------------|--------------|--------------|-------------|---|
| 1   | A     | 41/50 (82%)    | 25±1 (60±3%) | 16±1 (40±3%) | 0           | 6 |
| All | All   | 820/1000 (82%) | 495 (60%)    | 325 (40%)    | 0           | 6 |

All 30 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     | 14  | LYS  | 20             |
| 1   | A     | 23  | THR  | 20             |
| 1   | A     | 24  | CYS  | 20             |
| 1   | A     | 35  | CYS  | 20             |
| 1   | A     | 42  | PHE  | 20             |
| 1   | A     | 10  | THR  | 19             |
| 1   | A     | 25  | SER  | 19             |
| 1   | A     | 45  | SER  | 19             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 2   | ILE  | 18             |
| 1   | A     | 44  | VAL  | 18             |
| 1   | A     | 9   | GLU  | 17             |
| 1   | A     | 48  | CYS  | 12             |
| 1   | A     | 51  | MET  | 12             |
| 1   | A     | 41  | SER  | 10             |
| 1   | A     | 8   | SER  | 9              |
| 1   | A     | 4   | ASP  | 8              |
| 1   | A     | 22  | ASP  | 8              |
| 1   | A     | 16  | ASP  | 8              |
| 1   | A     | 3   | GLU  | 7              |
| 1   | A     | 30  | ASN  | 6              |
| 1   | A     | 19  | LEU  | 6              |
| 1   | A     | 40  | PHE  | 5              |
| 1   | A     | 46  | GLN  | 5              |
| 1   | A     | 47  | SER  | 5              |
| 1   | A     | 38  | GLN  | 4              |
| 1   | A     | 15  | ASN  | 3              |
| 1   | A     | 39  | CYS  | 3              |
| 1   | A     | 36  | CYS  | 2              |
| 1   | A     | 17  | SER  | 1              |
| 1   | A     | 18  | GLN  | 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 60% for the well-defined parts and 59% 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                  | 389 |
| Number of shifts mapped to atoms        | 389 |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 0   |
| Number of shifts with mapping warnings  | 0   |
| Number of shift outliers (ShiftChecker) | 1   |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 48       | $-0.37 \pm 0.31$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 4        | —                               | None (insufficient data)   |
| $^{13}\text{C}'$       | 0        | —                               | None (insufficient data)   |
| $^{15}\text{N}$        | 0        | —                               | None (insufficient data)   |

#### 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 60%, i.e. 330 atoms were assigned a chemical shift out of a possible 550. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 137/240 (57%) | 98/98 (100%)  | 39/96 (41%)     | 0/46 (0%)       |
| Sidechain | 165/250 (66%) | 149/162 (92%) | 16/82 (20%)     | 0/6 (0%)        |

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|          | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|---------------|----------------|-----------------|-----------------|
| Aromatic | 28/60 (47%)   | 28/29 (97%)    | 0/30 (0%)       | 0/1 (0%)        |
| Overall  | 330/550 (60%) | 275/289 (95%)  | 55/208 (26%)    | 0/53 (0%)       |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 59%, i.e. 389 atoms were assigned a chemical shift out of a possible 661. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 169/300 (56%) | 121/123 (98%)  | 48/120 (40%)    | 0/57 (0%)       |
| Sidechain | 192/301 (64%) | 174/193 (90%)  | 18/100 (18%)    | 0/8 (0%)        |
| Aromatic  | 28/60 (47%)   | 28/29 (97%)    | 0/30 (0%)       | 0/1 (0%)        |
| Overall   | 389/661 (59%) | 323/345 (94%)  | 66/250 (26%)    | 0/66 (0%)       |

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

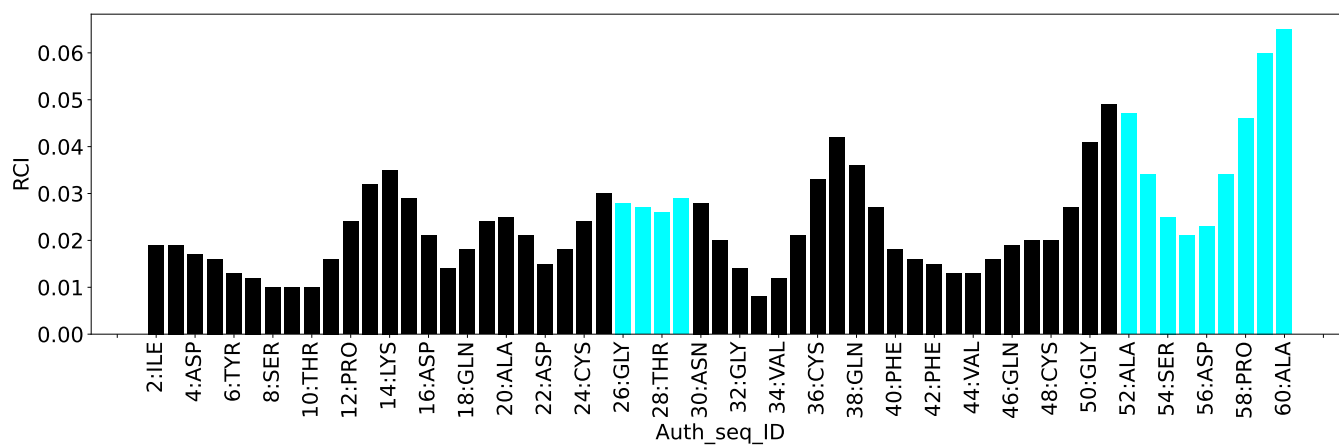
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 25  | SER  | HB3  | 2.42       | 2.49 – 5.20         | -5.2    |

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 699   |
| Intra-residue ( $ i-j =0$ )                              | 164   |
| Sequential ( $ i-j =1$ )                                 | 210   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 116   |
| Long range ( $ i-j \geq 5$ )                             | 205   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 4     |
| Total dihedral-angle restraints                          | 0     |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 11.7  |
| Number of long range restraints per residue <sup>1</sup> | 3.5   |

<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)  | 9.8                                    | 0.2     |
| 0.2-0.5 (Medium) | 13.3                                   | 0.5     |
| >0.5 (Large)     | 20.3                                   | 2.28    |

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

Dihedral-angle violations less than  $1^\circ$  are not included in the calculation. There are no dihedral-angle violations

## 9 Distance violation analysis ⓘ

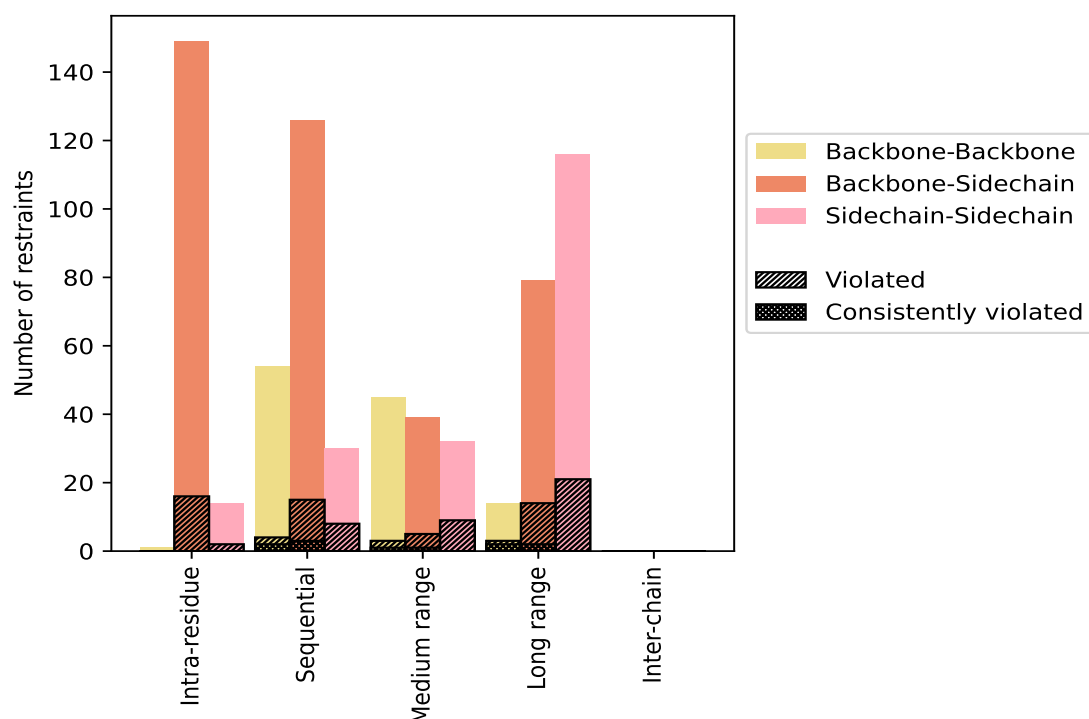
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                                              | Count      | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|-----------------------------------------------------------------------------|------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                                                             |            |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>164</b> | <b>23.5</b>    | <b>18</b>             | <b>11.0</b>    | <b>2.6</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 1          | 0.1            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 149        | 21.3           | 16                    | 10.7           | 2.3            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 14         | 2.0            | 2                     | 14.3           | 0.3            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>210</b> | <b>30.0</b>    | <b>27</b>             | <b>12.9</b>    | <b>3.9</b>     | <b>5</b>                           | <b>2.4</b>     | <b>0.7</b>     |
| Backbone-Backbone                                                           | 54         | 7.7            | 4                     | 7.4            | 0.6            | 2                                  | 3.7            | 0.3            |
| Backbone-Sidechain                                                          | 126        | 18.0           | 15                    | 11.9           | 2.1            | 3                                  | 2.4            | 0.4            |
| Sidechain-Sidechain                                                         | 30         | 4.3            | 8                     | 26.7           | 1.1            | 0                                  | 0.0            | 0.0            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>116</b> | <b>16.6</b>    | <b>17</b>             | <b>14.7</b>    | <b>2.4</b>     | <b>2</b>                           | <b>1.7</b>     | <b>0.3</b>     |
| Backbone-Backbone                                                           | 45         | 6.4            | 3                     | 6.7            | 0.4            | 1                                  | 2.2            | 0.1            |
| Backbone-Sidechain                                                          | 39         | 5.6            | 5                     | 12.8           | 0.7            | 1                                  | 2.6            | 0.1            |
| Sidechain-Sidechain                                                         | 32         | 4.6            | 9                     | 28.1           | 1.3            | 0                                  | 0.0            | 0.0            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>205</b> | <b>29.3</b>    | <b>38</b>             | <b>18.5</b>    | <b>5.4</b>     | <b>4</b>                           | <b>2.0</b>     | <b>0.6</b>     |
| Backbone-Backbone                                                           | 14         | 2.0            | 3                     | 21.4           | 0.4            | 2                                  | 14.3           | 0.3            |
| Backbone-Sidechain                                                          | 79         | 11.3           | 14                    | 17.7           | 2.0            | 2                                  | 2.5            | 0.3            |
| Sidechain-Sidechain                                                         | 112        | 16.0           | 21                    | 18.8           | 3.0            | 0                                  | 0.0            | 0.0            |
| <b>Inter-chain</b>                                                          | <b>0</b>   | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 0          | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 0          | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 0          | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>                                                        | <b>0</b>   | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>                                                       | <b>4</b>   | <b>0.6</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>                                                                | <b>699</b> | <b>100.0</b>   | <b>100</b>            | <b>14.3</b>    | <b>14.3</b>    | <b>11</b>                          | <b>1.6</b>     | <b>1.6</b>     |
| Backbone-Backbone                                                           | 114        | 16.3           | 10                    | 8.8            | 1.4            | 5                                  | 4.4            | 0.7            |
| Backbone-Sidechain                                                          | 393        | 56.2           | 50                    | 12.7           | 7.2            | 6                                  | 1.5            | 0.9            |
| Sidechain-Sidechain                                                         | 192        | 27.5           | 40                    | 20.8           | 5.7            | 0                                  | 0.0            | 0.0            |

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

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



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

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 6                    | 9               | 8               | 21              | 0               | 44    | 0.65     | 2.16    | 0.5                 | 0.47       |
| 2        | 6                    | 12              | 7               | 21              | 0               | 46    | 0.66     | 2.19    | 0.49                | 0.52       |
| 3        | 4                    | 12              | 6               | 15              | 0               | 37    | 0.53     | 1.72    | 0.39                | 0.45       |
| 4        | 6                    | 14              | 7               | 18              | 0               | 45    | 0.66     | 2.21    | 0.48                | 0.5        |
| 5        | 7                    | 12              | 4               | 15              | 0               | 38    | 0.52     | 1.77    | 0.38                | 0.46       |
| 6        | 6                    | 13              | 9               | 20              | 0               | 48    | 0.6      | 2.16    | 0.47                | 0.48       |
| 7        | 7                    | 10              | 5               | 16              | 0               | 38    | 0.55     | 2.06    | 0.45                | 0.4        |
| 8        | 7                    | 12              | 5               | 17              | 0               | 41    | 0.55     | 1.76    | 0.41                | 0.45       |
| 9        | 7                    | 10              | 9               | 18              | 0               | 44    | 0.6      | 1.76    | 0.49                | 0.43       |
| 10       | 7                    | 12              | 3               | 15              | 0               | 37    | 0.59     | 1.79    | 0.42                | 0.52       |

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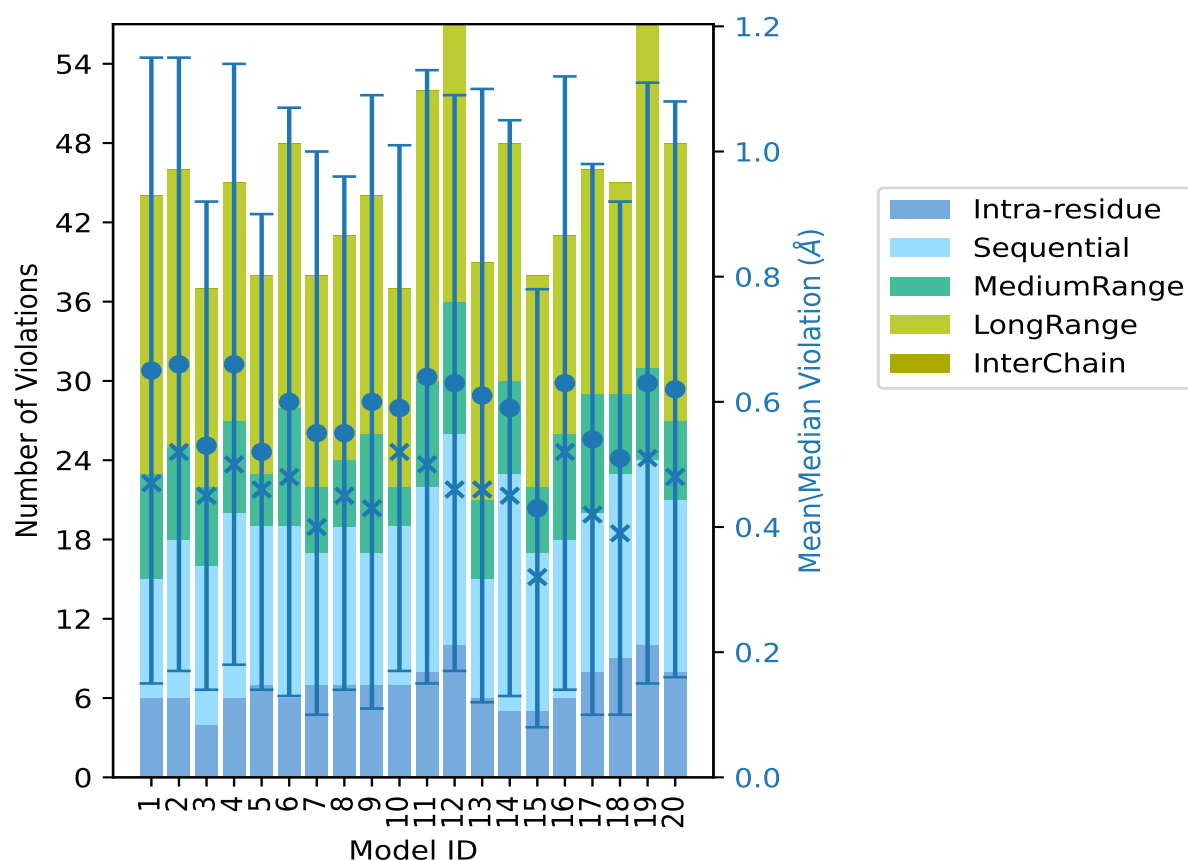
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 8                    | 14              | 8               | 22              | 0               | 52    | 0.64     | 2.23    | 0.49                | 0.5        |
| 12       | 10                   | 16              | 10              | 21              | 0               | 57    | 0.63     | 2.03    | 0.46                | 0.46       |
| 13       | 6                    | 9               | 6               | 18              | 0               | 39    | 0.61     | 2.16    | 0.49                | 0.46       |
| 14       | 5                    | 18              | 7               | 18              | 0               | 48    | 0.59     | 2.05    | 0.46                | 0.45       |
| 15       | 5                    | 12              | 5               | 16              | 0               | 38    | 0.43     | 1.74    | 0.35                | 0.32       |
| 16       | 6                    | 12              | 8               | 15              | 0               | 41    | 0.63     | 1.75    | 0.49                | 0.52       |
| 17       | 8                    | 12              | 9               | 17              | 0               | 46    | 0.54     | 2.0     | 0.44                | 0.42       |
| 18       | 9                    | 14              | 6               | 16              | 0               | 45    | 0.51     | 1.66    | 0.41                | 0.39       |
| 19       | 10                   | 14              | 7               | 26              | 0               | 57    | 0.63     | 2.22    | 0.48                | 0.51       |
| 20       | 8                    | 13              | 6               | 21              | 0               | 48    | 0.62     | 2.28    | 0.46                | 0.48       |

<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

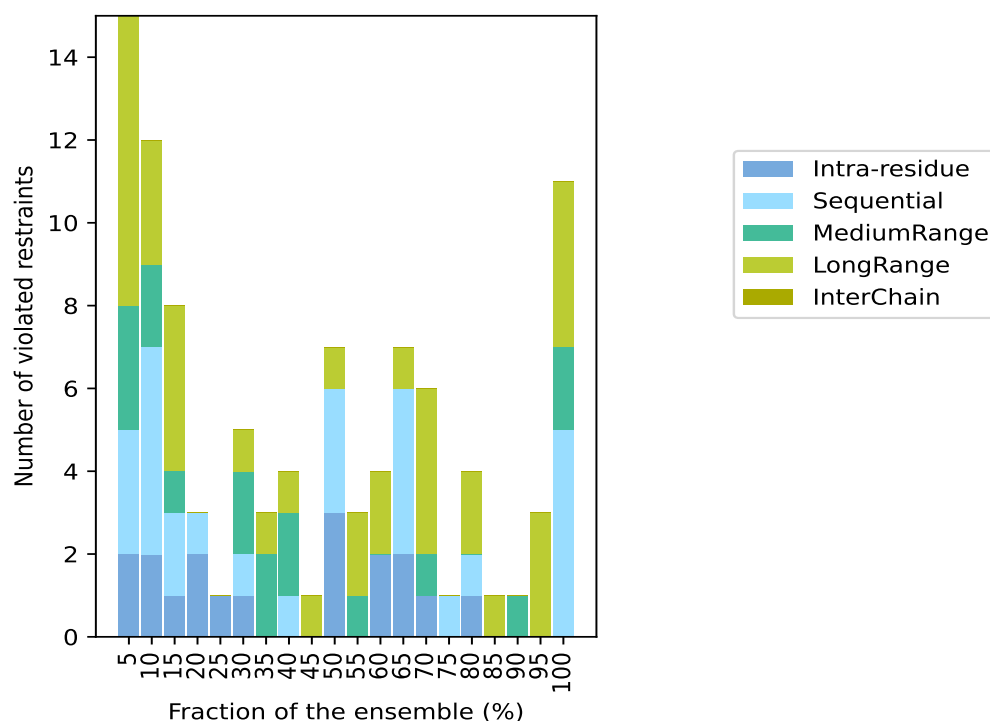
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 595(IR:146, SQ:183, MR:99, LR:167, IC:0) restraints are not 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>       | %     |
| 2                             | 3               | 3               | 7               | 0               | 15    | 1                        | 5.0   |
| 2                             | 5               | 2               | 3               | 0               | 12    | 2                        | 10.0  |
| 1                             | 2               | 1               | 4               | 0               | 8     | 3                        | 15.0  |
| 2                             | 1               | 0               | 0               | 0               | 3     | 4                        | 20.0  |
| 1                             | 0               | 0               | 0               | 0               | 1     | 5                        | 25.0  |
| 1                             | 1               | 2               | 1               | 0               | 5     | 6                        | 30.0  |
| 0                             | 0               | 2               | 1               | 0               | 3     | 7                        | 35.0  |
| 0                             | 1               | 2               | 1               | 0               | 4     | 8                        | 40.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 9                        | 45.0  |
| 3                             | 3               | 0               | 1               | 0               | 7     | 10                       | 50.0  |
| 0                             | 0               | 1               | 2               | 0               | 3     | 11                       | 55.0  |
| 2                             | 0               | 0               | 2               | 0               | 4     | 12                       | 60.0  |
| 2                             | 4               | 0               | 1               | 0               | 7     | 13                       | 65.0  |
| 1                             | 0               | 1               | 4               | 0               | 6     | 14                       | 70.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 15                       | 75.0  |
| 1                             | 1               | 0               | 2               | 0               | 4     | 16                       | 80.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 17                       | 85.0  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 18                       | 90.0  |
| 0                             | 0               | 0               | 3               | 0               | 3     | 19                       | 95.0  |
| 0                             | 5               | 2               | 4               | 0               | 11    | 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

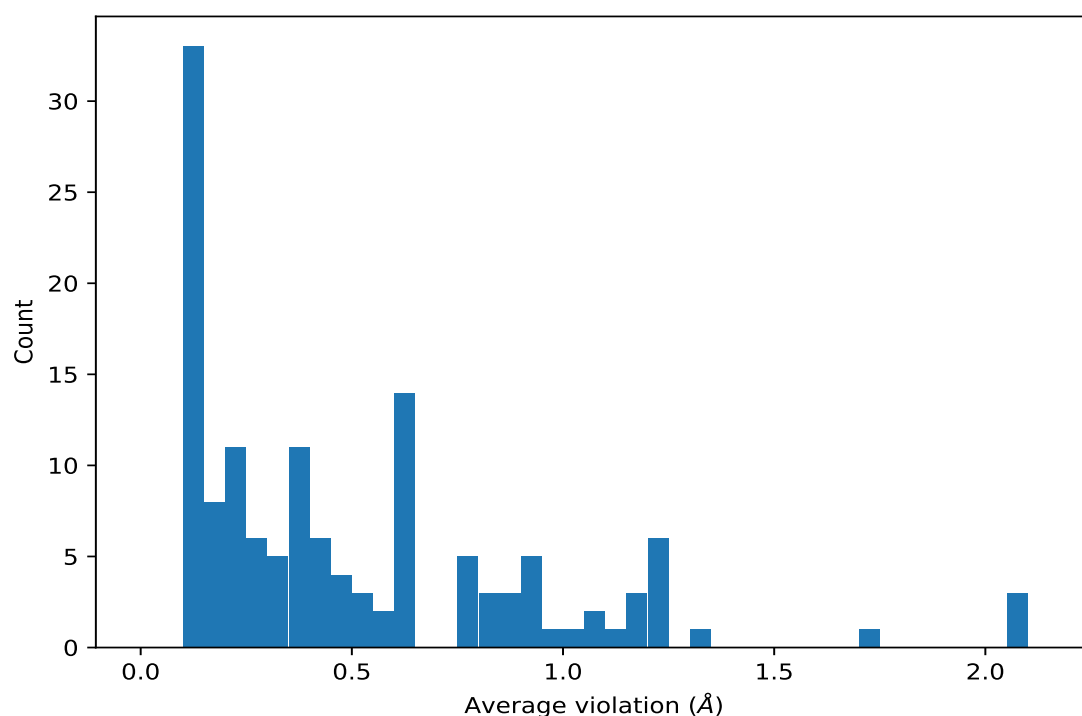
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|---------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,558) | 1:47:A:SER:HA  | 1:50:A:GLY:HA2  | 20                  | 1.74     | 0.05                | 1.74       |
| (1,262) | 1:21:A:TRP:HA  | 1:24:A:CYS:HB2  | 20                  | 1.3      | 0.24                | 1.31       |
| (1,162) | 1:32:A:GLY:HA3 | 1:49:A:ALA:HA   | 20                  | 1.07     | 0.06                | 1.08       |
| (1,266) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HA   | 20                  | 0.9      | 0.29                | 0.93       |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG21 | 20                  | 0.79     | 0.08                | 0.8        |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG22 | 20                  | 0.79     | 0.08                | 0.8        |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG23 | 20                  | 0.79     | 0.08                | 0.8        |
| (1,574) | 1:25:A:SER:HB2 | 1:48:A:CYS:HA   | 20                  | 0.63     | 0.11                | 0.66       |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB2  | 20                  | 0.62     | 0.13                | 0.61       |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB3  | 20                  | 0.62     | 0.13                | 0.61       |
| (1,243) | 1:11:A:CYS:H   | 1:12:A:PRO:HD2  | 20                  | 0.46     | 0.0                 | 0.46       |
| (1,104) | 1:44:A:VAL:H   | 1:45:A:SER:HA   | 20                  | 0.34     | 0.01                | 0.34       |
| (1,248) | 1:5:A:PHE:HB3  | 1:6:A:TYR:H     | 20                  | 0.21     | 0.02                | 0.2        |
| (1,547) | 1:53:A:ASP:HA  | 1:54:A:SER:HA   | 20                  | 0.12     | 0.02                | 0.12       |
| (1,282) | 1:25:A:SER:HB2 | 1:52:A:ALA:H    | 19                  | 0.79     | 0.16                | 0.73       |
| (1,373) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HB2  | 19                  | 0.47     | 0.15                | 0.5        |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,373) | 1:12:A:PRO:HD2  | 1:38:A:GLN:HB3  | 19                  | 0.47     | 0.15                | 0.5        |
| (1,370) | 1:40:A:PHE:HB3  | 1:45:A:SER:HB2  | 19                  | 0.16     | 0.03                | 0.16       |
| (1,370) | 1:40:A:PHE:HB3  | 1:45:A:SER:HB3  | 19                  | 0.16     | 0.03                | 0.16       |
| (1,354) | 1:16:A:ASP:HB2  | 1:19:A:LEU:HD11 | 18                  | 0.82     | 0.24                | 0.86       |
| (1,354) | 1:16:A:ASP:HB2  | 1:19:A:LEU:HD12 | 18                  | 0.82     | 0.24                | 0.86       |
| (1,354) | 1:16:A:ASP:HB2  | 1:19:A:LEU:HD13 | 18                  | 0.82     | 0.24                | 0.86       |
| (1,581) | 1:3:A:GLU:HB2   | 1:17:A:SER:HB2  | 17                  | 1.02     | 0.49                | 1.21       |
| (1,242) | 1:17:A:SER:HB3  | 1:18:A:GLN:HA   | 16                  | 1.14     | 0.02                | 1.14       |
| (1,511) | 1:2:A:ILE:HG21  | 1:17:A:SER:HB3  | 16                  | 0.62     | 0.1                 | 0.6        |
| (1,511) | 1:2:A:ILE:HG22  | 1:17:A:SER:HB3  | 16                  | 0.62     | 0.1                 | 0.6        |
| (1,511) | 1:2:A:ILE:HG23  | 1:17:A:SER:HB3  | 16                  | 0.62     | 0.1                 | 0.6        |
| (1,605) | 1:27:A:GLY:HA3  | 1:53:A:ASP:HB2  | 16                  | 0.42     | 0.13                | 0.43       |
| (1,605) | 1:27:A:GLY:HA3  | 1:53:A:ASP:HB3  | 16                  | 0.42     | 0.13                | 0.43       |
| (1,285) | 1:17:A:SER:H    | 1:17:A:SER:HB2  | 16                  | 0.38     | 0.03                | 0.38       |
| (1,281) | 1:12:A:PRO:HD3  | 1:13:A:TYR:HE1  | 15                  | 0.59     | 0.3                 | 0.58       |
| (1,281) | 1:12:A:PRO:HD3  | 1:13:A:TYR:HE2  | 15                  | 0.59     | 0.3                 | 0.58       |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD11 | 14                  | 2.08     | 0.18                | 2.16       |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD12 | 14                  | 2.08     | 0.18                | 2.16       |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD13 | 14                  | 2.08     | 0.18                | 2.16       |
| (1,496) | 1:19:A:LEU:HD21 | 1:22:A:ASP:HB3  | 14                  | 1.21     | 0.35                | 1.23       |
| (1,496) | 1:19:A:LEU:HD22 | 1:22:A:ASP:HB3  | 14                  | 1.21     | 0.35                | 1.23       |
| (1,496) | 1:19:A:LEU:HD23 | 1:22:A:ASP:HB3  | 14                  | 1.21     | 0.35                | 1.23       |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD11 | 14                  | 1.2      | 0.33                | 1.29       |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD12 | 14                  | 1.2      | 0.33                | 1.29       |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD13 | 14                  | 1.2      | 0.33                | 1.29       |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD11 | 14                  | 0.88     | 0.44                | 0.94       |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD12 | 14                  | 0.88     | 0.44                | 0.94       |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD13 | 14                  | 0.88     | 0.44                | 0.94       |
| (1,478) | 1:13:A:TYR:HB3  | 1:19:A:LEU:HD11 | 14                  | 0.62     | 0.27                | 0.72       |
| (1,478) | 1:13:A:TYR:HB3  | 1:19:A:LEU:HD12 | 14                  | 0.62     | 0.27                | 0.72       |
| (1,478) | 1:13:A:TYR:HB3  | 1:19:A:LEU:HD13 | 14                  | 0.62     | 0.27                | 0.72       |
| (1,80)  | 1:35:A:CYS:H    | 1:35:A:CYS:HB2  | 14                  | 0.12     | 0.02                | 0.12       |
| (1,512) | 1:2:A:ILE:HG21  | 1:3:A:GLU:HB2   | 13                  | 1.19     | 0.02                | 1.19       |
| (1,512) | 1:2:A:ILE:HG22  | 1:3:A:GLU:HB2   | 13                  | 1.19     | 0.02                | 1.19       |
| (1,512) | 1:2:A:ILE:HG23  | 1:3:A:GLU:HB2   | 13                  | 1.19     | 0.02                | 1.19       |
| (1,94)  | 1:46:A:GLN:HG3  | 1:47:A:SER:H    | 13                  | 0.6      | 0.09                | 0.62       |
| (1,402) | 1:3:A:GLU:H     | 1:3:A:GLU:HB2   | 13                  | 0.45     | 0.0                 | 0.45       |
| (1,594) | 1:56:A:ASP:HA   | 1:56:A:ASP:HB2  | 13                  | 0.27     | 0.02                | 0.28       |
| (1,414) | 1:3:A:GLU:HB3   | 1:4:A:ASP:H     | 13                  | 0.21     | 0.04                | 0.22       |
| (1,175) | 1:52:A:ALA:HB1  | 1:53:A:ASP:HA   | 13                  | 0.14     | 0.02                | 0.14       |
| (1,175) | 1:52:A:ALA:HB2  | 1:53:A:ASP:HA   | 13                  | 0.14     | 0.02                | 0.14       |
| (1,175) | 1:52:A:ALA:HB3  | 1:53:A:ASP:HA   | 13                  | 0.14     | 0.02                | 0.14       |

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| Key     | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,692) | 1:35:A:CYS:SG  | 1:48:A:CYS:CB   | 13                  | 0.13     | 0.02                | 0.13       |
| (1,583) | 1:36:A:CYS:HB2 | 1:45:A:SER:HA   | 12                  | 0.97     | 0.02                | 0.96       |
| (1,320) | 1:36:A:CYS:H   | 1:36:A:CYS:HB3  | 12                  | 0.52     | 0.0                 | 0.52       |
| (1,384) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HG2  | 12                  | 0.5      | 0.22                | 0.43       |
| (1,384) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HG3  | 12                  | 0.5      | 0.22                | 0.43       |
| (1,618) | 1:3:A:GLU:HB2  | 1:3:A:GLU:HG2   | 12                  | 0.26     | 0.05                | 0.28       |
| (1,477) | 1:13:A:TYR:HD1 | 1:19:A:LEU:HD11 | 11                  | 0.38     | 0.16                | 0.33       |
| (1,477) | 1:13:A:TYR:HD1 | 1:19:A:LEU:HD12 | 11                  | 0.38     | 0.16                | 0.33       |
| (1,477) | 1:13:A:TYR:HD1 | 1:19:A:LEU:HD13 | 11                  | 0.38     | 0.16                | 0.33       |
| (1,477) | 1:13:A:TYR:HD2 | 1:19:A:LEU:HD11 | 11                  | 0.38     | 0.16                | 0.33       |
| (1,477) | 1:13:A:TYR:HD2 | 1:19:A:LEU:HD12 | 11                  | 0.38     | 0.16                | 0.33       |
| (1,477) | 1:13:A:TYR:HD2 | 1:19:A:LEU:HD13 | 11                  | 0.38     | 0.16                | 0.33       |
| (1,541) | 1:6:A:TYR:HA   | 1:17:A:SER:HB2  | 11                  | 0.27     | 0.19                | 0.18       |
| (1,74)  | 1:16:A:ASP:HB2 | 1:18:A:GLN:H    | 11                  | 0.2      | 0.07                | 0.19       |
| (1,186) | 1:14:A:LYS:HA  | 1:14:A:LYS:HD2  | 10                  | 1.06     | 0.02                | 1.06       |
| (1,14)  | 1:14:A:LYS:HD2 | 1:15:A:ASN:H    | 10                  | 0.94     | 0.28                | 1.06       |
| (1,482) | 1:7:A:THR:HG21 | 1:41:A:SER:HB3  | 10                  | 0.9      | 0.07                | 0.88       |
| (1,482) | 1:7:A:THR:HG22 | 1:41:A:SER:HB3  | 10                  | 0.9      | 0.07                | 0.88       |
| (1,482) | 1:7:A:THR:HG23 | 1:41:A:SER:HB3  | 10                  | 0.9      | 0.07                | 0.88       |
| (1,199) | 1:41:A:SER:HB2 | 1:42:A:PHE:H    | 10                  | 0.78     | 0.02                | 0.78       |
| (1,436) | 1:14:A:LYS:HB2 | 1:14:A:LYS:HD2  | 10                  | 0.44     | 0.03                | 0.45       |
| (1,436) | 1:14:A:LYS:HB3 | 1:14:A:LYS:HD2  | 10                  | 0.44     | 0.03                | 0.45       |
| (1,360) | 1:22:A:ASP:HB2 | 1:23:A:THR:H    | 10                  | 0.43     | 0.21                | 0.49       |
| (1,550) | 1:41:A:SER:HA  | 1:41:A:SER:HB2  | 10                  | 0.33     | 0.01                | 0.34       |
| (1,579) | 1:6:A:TYR:HD1  | 1:17:A:SER:HB2  | 9                   | 0.32     | 0.1                 | 0.36       |
| (1,579) | 1:6:A:TYR:HD2  | 1:17:A:SER:HB2  | 9                   | 0.32     | 0.1                 | 0.36       |
| (1,377) | 1:4:A:ASP:HB2  | 1:5:A:PHE:HE1   | 8                   | 0.63     | 0.01                | 0.63       |
| (1,377) | 1:4:A:ASP:HB2  | 1:5:A:PHE:HE2   | 8                   | 0.63     | 0.01                | 0.63       |
| (1,481) | 1:16:A:ASP:HB3 | 1:19:A:LEU:HD11 | 8                   | 0.39     | 0.26                | 0.3        |
| (1,481) | 1:16:A:ASP:HB3 | 1:19:A:LEU:HD12 | 8                   | 0.39     | 0.26                | 0.3        |
| (1,481) | 1:16:A:ASP:HB3 | 1:19:A:LEU:HD13 | 8                   | 0.39     | 0.26                | 0.3        |
| (1,639) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HB2  | 8                   | 0.26     | 0.07                | 0.28       |
| (1,575) | 1:6:A:TYR:HE1  | 1:17:A:SER:HB2  | 8                   | 0.21     | 0.08                | 0.2        |
| (1,575) | 1:6:A:TYR:HE2  | 1:17:A:SER:HB2  | 8                   | 0.21     | 0.08                | 0.2        |
| (1,251) | 1:26:A:GLY:HA2 | 1:28:A:THR:H    | 7                   | 0.64     | 0.35                | 0.66       |
| (1,607) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HB3  | 7                   | 0.43     | 0.12                | 0.44       |
| (1,50)  | 1:25:A:SER:HA  | 1:52:A:ALA:H    | 7                   | 0.12     | 0.02                | 0.12       |
| (1,536) | 1:21:A:TRP:HZ3 | 1:25:A:SER:HB2  | 6                   | 0.26     | 0.13                | 0.22       |
| (1,385) | 1:3:A:GLU:H    | 1:3:A:GLU:HG2   | 6                   | 0.25     | 0.1                 | 0.32       |
| (1,366) | 1:24:A:CYS:HB3 | 1:35:A:CYS:HB2  | 6                   | 0.21     | 0.1                 | 0.19       |
| (1,566) | 1:34:A:VAL:HA  | 1:38:A:GLN:HB2  | 6                   | 0.19     | 0.01                | 0.18       |
| (1,566) | 1:34:A:VAL:HA  | 1:38:A:GLN:HB3  | 6                   | 0.19     | 0.01                | 0.18       |

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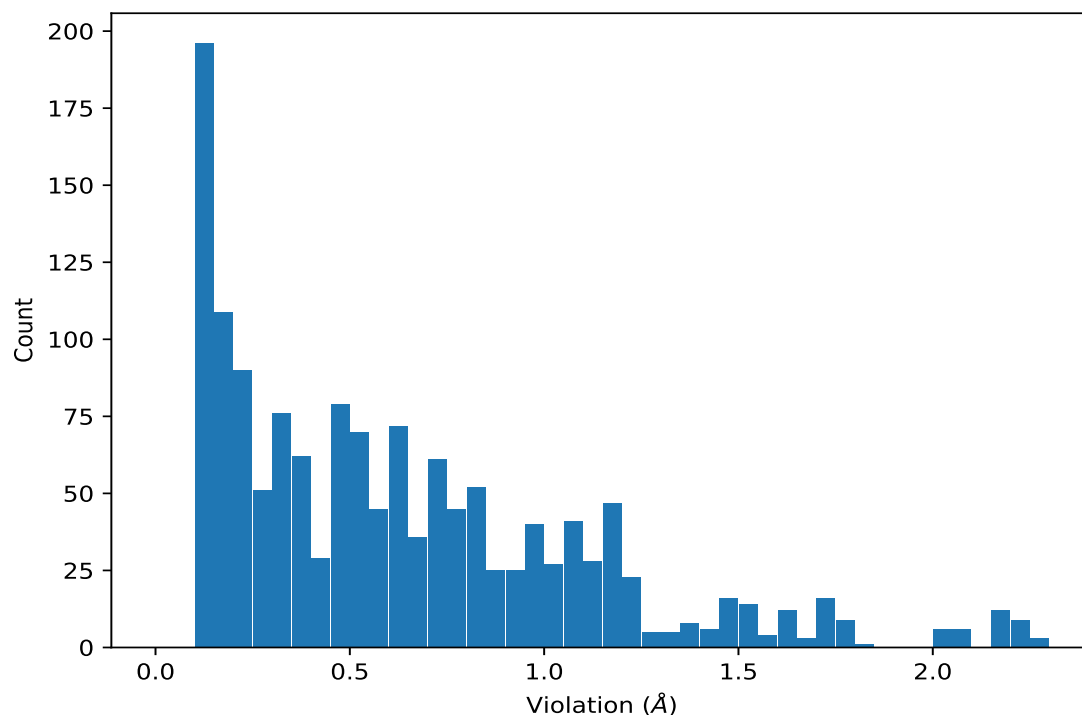
| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,641) | 1:19:A:LEU:HB3  | 1:20:A:ALA:HA   | 6                   | 0.15     | 0.02                | 0.14       |
| (1,559) | 1:54:A:SER:HA   | 1:54:A:SER:HB2  | 5                   | 0.11     | 0.0                 | 0.11       |
| (1,45)  | 1:15:A:ASN:HB2  | 1:16:A:ASP:H    | 4                   | 0.36     | 0.01                | 0.36       |
| (1,614) | 1:46:A:GLN:HA   | 1:46:A:GLN:HG2  | 4                   | 0.3      | 0.01                | 0.3        |
| (1,294) | 1:17:A:SER:HA   | 1:17:A:SER:HB3  | 4                   | 0.24     | 0.01                | 0.24       |
| (1,98)  | 1:51:A:MET:HG3  | 1:53:A:ASP:H    | 3                   | 0.63     | 0.68                | 0.2        |
| (1,688) | 1:11:A:CYS:SG   | 1:39:A:CYS:CB   | 3                   | 0.23     | 0.01                | 0.22       |
| (1,554) | 1:19:A:LEU:HD11 | 1:20:A:ALA:HA   | 3                   | 0.17     | 0.05                | 0.2        |
| (1,554) | 1:19:A:LEU:HD12 | 1:20:A:ALA:HA   | 3                   | 0.17     | 0.05                | 0.2        |
| (1,554) | 1:19:A:LEU:HD13 | 1:20:A:ALA:HA   | 3                   | 0.17     | 0.05                | 0.2        |
| (1,565) | 1:36:A:CYS:HB3  | 1:45:A:SER:HA   | 3                   | 0.14     | 0.03                | 0.13       |
| (1,46)  | 1:37:A:GLY:H    | 1:45:A:SER:HB2  | 3                   | 0.13     | 0.01                | 0.13       |
| (1,46)  | 1:37:A:GLY:H    | 1:45:A:SER:HB3  | 3                   | 0.13     | 0.01                | 0.13       |
| (1,198) | 1:41:A:SER:H    | 1:41:A:SER:HB2  | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,609) | 1:11:A:CYS:HA   | 1:38:A:GLN:HB2  | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,609) | 1:11:A:CYS:HA   | 1:38:A:GLN:HB3  | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,155) | 1:41:A:SER:HA   | 1:42:A:PHE:HB3  | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,601) | 1:23:A:THR:HG21 | 1:30:A:ASN:HB2  | 2                   | 0.24     | 0.01                | 0.24       |
| (1,601) | 1:23:A:THR:HG22 | 1:30:A:ASN:HB2  | 2                   | 0.24     | 0.01                | 0.24       |
| (1,601) | 1:23:A:THR:HG23 | 1:30:A:ASN:HB2  | 2                   | 0.24     | 0.01                | 0.24       |
| (1,279) | 1:12:A:PRO:HD3  | 1:13:A:TYR:HD1  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,279) | 1:12:A:PRO:HD3  | 1:13:A:TYR:HD2  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,353) | 1:6:A:TYR:HE1   | 1:39:A:CYS:HB3  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,353) | 1:6:A:TYR:HE2   | 1:39:A:CYS:HB3  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,669) | 1:21:A:TRP:HE3  | 1:44:A:VAL:HG11 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,669) | 1:21:A:TRP:HE3  | 1:44:A:VAL:HG12 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,669) | 1:21:A:TRP:HE3  | 1:44:A:VAL:HG13 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,318) | 1:14:A:LYS:HE3  | 1:15:A:ASN:HB2  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,43)  | 1:16:A:ASP:H    | 1:17:A:SER:HA   | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,181) | 1:9:A:GLU:HB3   | 1:10:A:THR:HB   | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,263) | 1:44:A:VAL:HA   | 1:48:A:CYS:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,612) | 1:30:A:ASN:HA   | 1:30:A:ASN:HB3  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,142) | 1:25:A:SER:H    | 1:26:A:GLY:H    | 2                   | 0.11     | 0.01                | 0.11       |
| (1,435) | 1:14:A:LYS:H    | 1:14:A:LYS:HB2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,435) | 1:14:A:LYS:H    | 1:14:A:LYS:HB3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,488) | 1:7:A:THR:HG21  | 1:11:A:CYS:H    | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,488) | 1:7:A:THR:HG22  | 1:11:A:CYS:H    | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,488) | 1:7:A:THR:HG23  | 1:11:A:CYS:H    | 2                   | 0.11     | 0.0                 | 0.11       |

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

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

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

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



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

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

| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,169) | 1:13:A:TYR:HA | 1:19:A:LEU:HD11 | 20       | 2.28          |
| (1,169) | 1:13:A:TYR:HA | 1:19:A:LEU:HD12 | 20       | 2.28          |
| (1,169) | 1:13:A:TYR:HA | 1:19:A:LEU:HD13 | 20       | 2.28          |
| (1,169) | 1:13:A:TYR:HA | 1:19:A:LEU:HD11 | 11       | 2.23          |
| (1,169) | 1:13:A:TYR:HA | 1:19:A:LEU:HD12 | 11       | 2.23          |
| (1,169) | 1:13:A:TYR:HA | 1:19:A:LEU:HD13 | 11       | 2.23          |
| (1,169) | 1:13:A:TYR:HA | 1:19:A:LEU:HD11 | 19       | 2.22          |
| (1,169) | 1:13:A:TYR:HA | 1:19:A:LEU:HD12 | 19       | 2.22          |
| (1,169) | 1:13:A:TYR:HA | 1:19:A:LEU:HD13 | 19       | 2.22          |
| (1,169) | 1:13:A:TYR:HA | 1:19:A:LEU:HD11 | 4        | 2.21          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD12 | 4        | 2.21          |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD13 | 4        | 2.21          |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD11 | 2        | 2.19          |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD12 | 2        | 2.19          |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD13 | 2        | 2.19          |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD11 | 1        | 2.16          |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD12 | 1        | 2.16          |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD13 | 1        | 2.16          |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD11 | 6        | 2.16          |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD12 | 6        | 2.16          |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD13 | 6        | 2.16          |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD11 | 13       | 2.16          |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD12 | 13       | 2.16          |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD13 | 13       | 2.16          |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD11 | 7        | 2.06          |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD12 | 7        | 2.06          |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD13 | 7        | 2.06          |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD11 | 14       | 2.05          |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD12 | 14       | 2.05          |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD13 | 14       | 2.05          |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD11 | 12       | 2.03          |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD12 | 12       | 2.03          |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD13 | 12       | 2.03          |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD11 | 17       | 2.0           |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD12 | 17       | 2.0           |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD13 | 17       | 2.0           |
| (1,558) | 1:47:A:SER:HA   | 1:50:A:GLY:HA2  | 19       | 1.82          |
| (1,558) | 1:47:A:SER:HA   | 1:50:A:GLY:HA2  | 6        | 1.79          |
| (1,558) | 1:47:A:SER:HA   | 1:50:A:GLY:HA2  | 10       | 1.79          |
| (1,558) | 1:47:A:SER:HA   | 1:50:A:GLY:HA2  | 5        | 1.77          |
| (1,558) | 1:47:A:SER:HA   | 1:50:A:GLY:HA2  | 13       | 1.77          |
| (1,558) | 1:47:A:SER:HA   | 1:50:A:GLY:HA2  | 20       | 1.77          |
| (1,558) | 1:47:A:SER:HA   | 1:50:A:GLY:HA2  | 8        | 1.76          |
| (1,558) | 1:47:A:SER:HA   | 1:50:A:GLY:HA2  | 9        | 1.76          |
| (1,558) | 1:47:A:SER:HA   | 1:50:A:GLY:HA2  | 12       | 1.76          |
| (1,558) | 1:47:A:SER:HA   | 1:50:A:GLY:HA2  | 16       | 1.75          |
| (1,558) | 1:47:A:SER:HA   | 1:50:A:GLY:HA2  | 4        | 1.74          |
| (1,558) | 1:47:A:SER:HA   | 1:50:A:GLY:HA2  | 15       | 1.74          |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD11 | 9        | 1.74          |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD12 | 9        | 1.74          |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD13 | 9        | 1.74          |
| (1,496) | 1:19:A:LEU:HD21 | 1:22:A:ASP:HB3  | 11       | 1.73          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,496) | 1:19:A:LEU:HD22 | 1:22:A:ASP:HB3  | 11       | 1.73          |
| (1,496) | 1:19:A:LEU:HD23 | 1:22:A:ASP:HB3  | 11       | 1.73          |
| (1,558) | 1:47:A:SER:HA   | 1:50:A:GLY:HA2  | 1        | 1.72          |
| (1,558) | 1:47:A:SER:HA   | 1:50:A:GLY:HA2  | 3        | 1.72          |
| (1,558) | 1:47:A:SER:HA   | 1:50:A:GLY:HA2  | 17       | 1.72          |
| (1,558) | 1:47:A:SER:HA   | 1:50:A:GLY:HA2  | 2        | 1.71          |
| (1,496) | 1:19:A:LEU:HD21 | 1:22:A:ASP:HB3  | 9        | 1.71          |
| (1,496) | 1:19:A:LEU:HD22 | 1:22:A:ASP:HB3  | 9        | 1.71          |
| (1,496) | 1:19:A:LEU:HD23 | 1:22:A:ASP:HB3  | 9        | 1.71          |
| (1,266) | 1:27:A:GLY:HA3  | 1:53:A:ASP:HA   | 19       | 1.7           |
| (1,558) | 1:47:A:SER:HA   | 1:50:A:GLY:HA2  | 11       | 1.66          |
| (1,558) | 1:47:A:SER:HA   | 1:50:A:GLY:HA2  | 14       | 1.66          |
| (1,558) | 1:47:A:SER:HA   | 1:50:A:GLY:HA2  | 18       | 1.66          |
| (1,558) | 1:47:A:SER:HA   | 1:50:A:GLY:HA2  | 7        | 1.64          |
| (1,262) | 1:21:A:TRP:HA   | 1:24:A:CYS:HB2  | 6        | 1.64          |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD11 | 16       | 1.64          |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD12 | 16       | 1.64          |
| (1,169) | 1:13:A:TYR:HA   | 1:19:A:LEU:HD13 | 16       | 1.64          |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD11 | 4        | 1.62          |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD12 | 4        | 1.62          |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD13 | 4        | 1.62          |
| (1,262) | 1:21:A:TRP:HA   | 1:24:A:CYS:HB2  | 16       | 1.61          |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD11 | 20       | 1.6           |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD12 | 20       | 1.6           |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD13 | 20       | 1.6           |
| (1,262) | 1:21:A:TRP:HA   | 1:24:A:CYS:HB2  | 12       | 1.59          |
| (1,98)  | 1:51:A:MET:HG3  | 1:53:A:ASP:H    | 1        | 1.59          |
| (1,262) | 1:21:A:TRP:HA   | 1:24:A:CYS:HB2  | 11       | 1.57          |
| (1,581) | 1:3:A:GLU:HB2   | 1:17:A:SER:HB2  | 16       | 1.55          |
| (1,581) | 1:3:A:GLU:HB2   | 1:17:A:SER:HB2  | 9        | 1.54          |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD11 | 1        | 1.53          |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD12 | 1        | 1.53          |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD13 | 1        | 1.53          |
| (1,581) | 1:3:A:GLU:HB2   | 1:17:A:SER:HB2  | 14       | 1.52          |
| (1,496) | 1:19:A:LEU:HD21 | 1:22:A:ASP:HB3  | 1        | 1.52          |
| (1,496) | 1:19:A:LEU:HD22 | 1:22:A:ASP:HB3  | 1        | 1.52          |
| (1,496) | 1:19:A:LEU:HD23 | 1:22:A:ASP:HB3  | 1        | 1.52          |
| (1,262) | 1:21:A:TRP:HA   | 1:24:A:CYS:HB2  | 8        | 1.52          |
| (1,581) | 1:3:A:GLU:HB2   | 1:17:A:SER:HB2  | 11       | 1.5           |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD11 | 4        | 1.5           |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD12 | 4        | 1.5           |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD13 | 4        | 1.5           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,262) | 1:21:A:TRP:HA   | 1:24:A:CYS:HB2  | 17       | 1.5           |
| (1,262) | 1:21:A:TRP:HA   | 1:24:A:CYS:HB2  | 19       | 1.49          |
| (1,496) | 1:19:A:LEU:HD21 | 1:22:A:ASP:HB3  | 13       | 1.48          |
| (1,496) | 1:19:A:LEU:HD22 | 1:22:A:ASP:HB3  | 13       | 1.48          |
| (1,496) | 1:19:A:LEU:HD23 | 1:22:A:ASP:HB3  | 13       | 1.48          |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD11 | 19       | 1.48          |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD12 | 19       | 1.48          |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD13 | 19       | 1.48          |
| (1,581) | 1:3:A:GLU:HB2   | 1:17:A:SER:HB2  | 2        | 1.47          |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD11 | 2        | 1.47          |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD12 | 2        | 1.47          |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD13 | 2        | 1.47          |
| (1,581) | 1:3:A:GLU:HB2   | 1:17:A:SER:HB2  | 12       | 1.46          |
| (1,496) | 1:19:A:LEU:HD21 | 1:22:A:ASP:HB3  | 7        | 1.46          |
| (1,496) | 1:19:A:LEU:HD22 | 1:22:A:ASP:HB3  | 7        | 1.46          |
| (1,496) | 1:19:A:LEU:HD23 | 1:22:A:ASP:HB3  | 7        | 1.46          |
| (1,262) | 1:21:A:TRP:HA   | 1:24:A:CYS:HB2  | 10       | 1.46          |
| (1,496) | 1:19:A:LEU:HD21 | 1:22:A:ASP:HB3  | 16       | 1.43          |
| (1,496) | 1:19:A:LEU:HD22 | 1:22:A:ASP:HB3  | 16       | 1.43          |
| (1,496) | 1:19:A:LEU:HD23 | 1:22:A:ASP:HB3  | 16       | 1.43          |
| (1,496) | 1:19:A:LEU:HD21 | 1:22:A:ASP:HB3  | 2        | 1.4           |
| (1,496) | 1:19:A:LEU:HD22 | 1:22:A:ASP:HB3  | 2        | 1.4           |
| (1,496) | 1:19:A:LEU:HD23 | 1:22:A:ASP:HB3  | 2        | 1.4           |
| (1,581) | 1:3:A:GLU:HB2   | 1:17:A:SER:HB2  | 4        | 1.38          |
| (1,262) | 1:21:A:TRP:HA   | 1:24:A:CYS:HB2  | 4        | 1.38          |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD11 | 1        | 1.37          |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD12 | 1        | 1.37          |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD13 | 1        | 1.37          |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD11 | 12       | 1.35          |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD12 | 12       | 1.35          |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD13 | 12       | 1.35          |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD11 | 11       | 1.33          |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD12 | 11       | 1.33          |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD13 | 11       | 1.33          |
| (1,262) | 1:21:A:TRP:HA   | 1:24:A:CYS:HB2  | 9        | 1.33          |
| (1,581) | 1:3:A:GLU:HB2   | 1:17:A:SER:HB2  | 19       | 1.31          |
| (1,262) | 1:21:A:TRP:HA   | 1:24:A:CYS:HB2  | 5        | 1.28          |
| (1,262) | 1:21:A:TRP:HA   | 1:24:A:CYS:HB2  | 18       | 1.28          |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD11 | 14       | 1.25          |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD12 | 14       | 1.25          |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD13 | 14       | 1.25          |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD11 | 6        | 1.24          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,480) | 1:13:A:TYR:HB2 | 1:19:A:LEU:HD12 | 6        | 1.24          |
| (1,480) | 1:13:A:TYR:HB2 | 1:19:A:LEU:HD13 | 6        | 1.24          |
| (1,479) | 1:14:A:LYS:HE2 | 1:19:A:LEU:HD11 | 13       | 1.24          |
| (1,479) | 1:14:A:LYS:HE2 | 1:19:A:LEU:HD12 | 13       | 1.24          |
| (1,479) | 1:14:A:LYS:HE2 | 1:19:A:LEU:HD13 | 13       | 1.24          |
| (1,266) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HA   | 12       | 1.24          |
| (1,480) | 1:13:A:TYR:HB2 | 1:19:A:LEU:HD11 | 13       | 1.23          |
| (1,480) | 1:13:A:TYR:HB2 | 1:19:A:LEU:HD12 | 13       | 1.23          |
| (1,480) | 1:13:A:TYR:HB2 | 1:19:A:LEU:HD13 | 13       | 1.23          |
| (1,581) | 1:3:A:GLU:HB2  | 1:17:A:SER:HB2  | 18       | 1.21          |
| (1,512) | 1:2:A:ILE:HG21 | 1:3:A:GLU:HB2   | 4        | 1.21          |
| (1,512) | 1:2:A:ILE:HG22 | 1:3:A:GLU:HB2   | 4        | 1.21          |
| (1,512) | 1:2:A:ILE:HG23 | 1:3:A:GLU:HB2   | 4        | 1.21          |
| (1,512) | 1:2:A:ILE:HG21 | 1:3:A:GLU:HB2   | 9        | 1.21          |
| (1,512) | 1:2:A:ILE:HG22 | 1:3:A:GLU:HB2   | 9        | 1.21          |
| (1,512) | 1:2:A:ILE:HG23 | 1:3:A:GLU:HB2   | 9        | 1.21          |
| (1,512) | 1:2:A:ILE:HG21 | 1:3:A:GLU:HB2   | 3        | 1.2           |
| (1,512) | 1:2:A:ILE:HG22 | 1:3:A:GLU:HB2   | 3        | 1.2           |
| (1,512) | 1:2:A:ILE:HG23 | 1:3:A:GLU:HB2   | 3        | 1.2           |
| (1,512) | 1:2:A:ILE:HG21 | 1:3:A:GLU:HB2   | 8        | 1.2           |
| (1,512) | 1:2:A:ILE:HG22 | 1:3:A:GLU:HB2   | 8        | 1.2           |
| (1,512) | 1:2:A:ILE:HG23 | 1:3:A:GLU:HB2   | 8        | 1.2           |
| (1,512) | 1:2:A:ILE:HG21 | 1:3:A:GLU:HB2   | 10       | 1.19          |
| (1,512) | 1:2:A:ILE:HG22 | 1:3:A:GLU:HB2   | 10       | 1.19          |
| (1,512) | 1:2:A:ILE:HG23 | 1:3:A:GLU:HB2   | 10       | 1.19          |
| (1,512) | 1:2:A:ILE:HG21 | 1:3:A:GLU:HB2   | 11       | 1.19          |
| (1,512) | 1:2:A:ILE:HG22 | 1:3:A:GLU:HB2   | 11       | 1.19          |
| (1,512) | 1:2:A:ILE:HG23 | 1:3:A:GLU:HB2   | 11       | 1.19          |
| (1,512) | 1:2:A:ILE:HG21 | 1:3:A:GLU:HB2   | 14       | 1.19          |
| (1,512) | 1:2:A:ILE:HG22 | 1:3:A:GLU:HB2   | 14       | 1.19          |
| (1,512) | 1:2:A:ILE:HG23 | 1:3:A:GLU:HB2   | 14       | 1.19          |
| (1,512) | 1:2:A:ILE:HG21 | 1:3:A:GLU:HB2   | 18       | 1.19          |
| (1,512) | 1:2:A:ILE:HG22 | 1:3:A:GLU:HB2   | 18       | 1.19          |
| (1,512) | 1:2:A:ILE:HG23 | 1:3:A:GLU:HB2   | 18       | 1.19          |
| (1,512) | 1:2:A:ILE:HG21 | 1:3:A:GLU:HB2   | 19       | 1.19          |
| (1,512) | 1:2:A:ILE:HG22 | 1:3:A:GLU:HB2   | 19       | 1.19          |
| (1,512) | 1:2:A:ILE:HG23 | 1:3:A:GLU:HB2   | 19       | 1.19          |
| (1,282) | 1:25:A:SER:HB2 | 1:52:A:ALA:H    | 19       | 1.19          |
| (1,266) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HA   | 14       | 1.19          |
| (1,512) | 1:2:A:ILE:HG21 | 1:3:A:GLU:HB2   | 12       | 1.18          |
| (1,512) | 1:2:A:ILE:HG22 | 1:3:A:GLU:HB2   | 12       | 1.18          |
| (1,512) | 1:2:A:ILE:HG23 | 1:3:A:GLU:HB2   | 12       | 1.18          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,512) | 1:2:A:ILE:HG21 | 1:3:A:GLU:HB2   | 16       | 1.18          |
| (1,512) | 1:2:A:ILE:HG22 | 1:3:A:GLU:HB2   | 16       | 1.18          |
| (1,512) | 1:2:A:ILE:HG23 | 1:3:A:GLU:HB2   | 16       | 1.18          |
| (1,479) | 1:14:A:LYS:HE2 | 1:19:A:LEU:HD11 | 6        | 1.18          |
| (1,479) | 1:14:A:LYS:HE2 | 1:19:A:LEU:HD12 | 6        | 1.18          |
| (1,479) | 1:14:A:LYS:HE2 | 1:19:A:LEU:HD13 | 6        | 1.18          |
| (1,242) | 1:17:A:SER:HB3 | 1:18:A:GLN:HA   | 12       | 1.18          |
| (1,512) | 1:2:A:ILE:HG21 | 1:3:A:GLU:HB2   | 2        | 1.17          |
| (1,512) | 1:2:A:ILE:HG22 | 1:3:A:GLU:HB2   | 2        | 1.17          |
| (1,512) | 1:2:A:ILE:HG23 | 1:3:A:GLU:HB2   | 2        | 1.17          |
| (1,242) | 1:17:A:SER:HB3 | 1:18:A:GLN:HA   | 19       | 1.17          |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD11 | 12       | 1.16          |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD12 | 12       | 1.16          |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD13 | 12       | 1.16          |
| (1,281) | 1:12:A:PRO:HD3 | 1:13:A:TYR:HE1  | 14       | 1.16          |
| (1,281) | 1:12:A:PRO:HD3 | 1:13:A:TYR:HE2  | 14       | 1.16          |
| (1,242) | 1:17:A:SER:HB3 | 1:18:A:GLN:HA   | 11       | 1.16          |
| (1,242) | 1:17:A:SER:HB3 | 1:18:A:GLN:HA   | 16       | 1.16          |
| (1,14)  | 1:14:A:LYS:HD2 | 1:15:A:ASN:H    | 19       | 1.16          |
| (1,512) | 1:2:A:ILE:HG21 | 1:3:A:GLU:HB2   | 20       | 1.15          |
| (1,512) | 1:2:A:ILE:HG22 | 1:3:A:GLU:HB2   | 20       | 1.15          |
| (1,512) | 1:2:A:ILE:HG23 | 1:3:A:GLU:HB2   | 20       | 1.15          |
| (1,266) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HA   | 10       | 1.15          |
| (1,262) | 1:21:A:TRP:HA  | 1:24:A:CYS:HB2  | 2        | 1.15          |
| (1,242) | 1:17:A:SER:HB3 | 1:18:A:GLN:HA   | 1        | 1.15          |
| (1,162) | 1:32:A:GLY:HA3 | 1:49:A:ALA:HA   | 20       | 1.15          |
| (1,14)  | 1:14:A:LYS:HD2 | 1:15:A:ASN:H    | 20       | 1.15          |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD11 | 9        | 1.14          |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD12 | 9        | 1.14          |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD13 | 9        | 1.14          |
| (1,242) | 1:17:A:SER:HB3 | 1:18:A:GLN:HA   | 3        | 1.14          |
| (1,242) | 1:17:A:SER:HB3 | 1:18:A:GLN:HA   | 4        | 1.14          |
| (1,242) | 1:17:A:SER:HB3 | 1:18:A:GLN:HA   | 5        | 1.14          |
| (1,242) | 1:17:A:SER:HB3 | 1:18:A:GLN:HA   | 6        | 1.14          |
| (1,242) | 1:17:A:SER:HB3 | 1:18:A:GLN:HA   | 9        | 1.14          |
| (1,242) | 1:17:A:SER:HB3 | 1:18:A:GLN:HA   | 14       | 1.14          |
| (1,242) | 1:17:A:SER:HB3 | 1:18:A:GLN:HA   | 18       | 1.14          |
| (1,242) | 1:17:A:SER:HB3 | 1:18:A:GLN:HA   | 2        | 1.13          |
| (1,242) | 1:17:A:SER:HB3 | 1:18:A:GLN:HA   | 15       | 1.13          |
| (1,162) | 1:32:A:GLY:HA3 | 1:49:A:ALA:HA   | 17       | 1.13          |
| (1,479) | 1:14:A:LYS:HE2 | 1:19:A:LEU:HD11 | 2        | 1.12          |
| (1,479) | 1:14:A:LYS:HE2 | 1:19:A:LEU:HD12 | 2        | 1.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD13 | 2        | 1.12          |
| (1,14)  | 1:14:A:LYS:HD2  | 1:15:A:ASN:H    | 12       | 1.12          |
| (1,581) | 1:3:A:GLU:HB2   | 1:17:A:SER:HB2  | 3        | 1.11          |
| (1,262) | 1:21:A:TRP:HA   | 1:24:A:CYS:HB2  | 13       | 1.11          |
| (1,162) | 1:32:A:GLY:HA3  | 1:49:A:ALA:HA   | 11       | 1.11          |
| (1,162) | 1:32:A:GLY:HA3  | 1:49:A:ALA:HA   | 12       | 1.11          |
| (1,14)  | 1:14:A:LYS:HD2  | 1:15:A:ASN:H    | 18       | 1.11          |
| (1,262) | 1:21:A:TRP:HA   | 1:24:A:CYS:HB2  | 7        | 1.1           |
| (1,262) | 1:21:A:TRP:HA   | 1:24:A:CYS:HB2  | 15       | 1.1           |
| (1,242) | 1:17:A:SER:HB3  | 1:18:A:GLN:HA   | 8        | 1.1           |
| (1,162) | 1:32:A:GLY:HA3  | 1:49:A:ALA:HA   | 5        | 1.1           |
| (1,162) | 1:32:A:GLY:HA3  | 1:49:A:ALA:HA   | 10       | 1.1           |
| (1,162) | 1:32:A:GLY:HA3  | 1:49:A:ALA:HA   | 13       | 1.1           |
| (1,354) | 1:16:A:ASP:HB2  | 1:19:A:LEU:HD11 | 16       | 1.09          |
| (1,354) | 1:16:A:ASP:HB2  | 1:19:A:LEU:HD12 | 16       | 1.09          |
| (1,354) | 1:16:A:ASP:HB2  | 1:19:A:LEU:HD13 | 16       | 1.09          |
| (1,266) | 1:27:A:GLY:HA3  | 1:53:A:ASP:HA   | 8        | 1.09          |
| (1,242) | 1:17:A:SER:HB3  | 1:18:A:GLN:HA   | 10       | 1.09          |
| (1,162) | 1:32:A:GLY:HA3  | 1:49:A:ALA:HA   | 9        | 1.09          |
| (1,14)  | 1:14:A:LYS:HD2  | 1:15:A:ASN:H    | 2        | 1.09          |
| (1,354) | 1:16:A:ASP:HB2  | 1:19:A:LEU:HD11 | 11       | 1.08          |
| (1,354) | 1:16:A:ASP:HB2  | 1:19:A:LEU:HD12 | 11       | 1.08          |
| (1,354) | 1:16:A:ASP:HB2  | 1:19:A:LEU:HD13 | 11       | 1.08          |
| (1,162) | 1:32:A:GLY:HA3  | 1:49:A:ALA:HA   | 4        | 1.08          |
| (1,162) | 1:32:A:GLY:HA3  | 1:49:A:ALA:HA   | 14       | 1.08          |
| (1,162) | 1:32:A:GLY:HA3  | 1:49:A:ALA:HA   | 18       | 1.08          |
| (1,162) | 1:32:A:GLY:HA3  | 1:49:A:ALA:HA   | 19       | 1.08          |
| (1,281) | 1:12:A:PRO:HD3  | 1:13:A:TYR:HE1  | 16       | 1.07          |
| (1,281) | 1:12:A:PRO:HD3  | 1:13:A:TYR:HE2  | 16       | 1.07          |
| (1,266) | 1:27:A:GLY:HA3  | 1:53:A:ASP:HA   | 6        | 1.07          |
| (1,186) | 1:14:A:LYS:HA   | 1:14:A:LYS:HD2  | 2        | 1.07          |
| (1,186) | 1:14:A:LYS:HA   | 1:14:A:LYS:HD2  | 11       | 1.07          |
| (1,186) | 1:14:A:LYS:HA   | 1:14:A:LYS:HD2  | 12       | 1.07          |
| (1,186) | 1:14:A:LYS:HA   | 1:14:A:LYS:HD2  | 18       | 1.07          |
| (1,186) | 1:14:A:LYS:HA   | 1:14:A:LYS:HD2  | 20       | 1.07          |
| (1,162) | 1:32:A:GLY:HA3  | 1:49:A:ALA:HA   | 6        | 1.07          |
| (1,162) | 1:32:A:GLY:HA3  | 1:49:A:ALA:HA   | 7        | 1.07          |
| (1,496) | 1:19:A:LEU:HD21 | 1:22:A:ASP:HB3  | 17       | 1.06          |
| (1,496) | 1:19:A:LEU:HD22 | 1:22:A:ASP:HB3  | 17       | 1.06          |
| (1,496) | 1:19:A:LEU:HD23 | 1:22:A:ASP:HB3  | 17       | 1.06          |
| (1,496) | 1:19:A:LEU:HD21 | 1:22:A:ASP:HB3  | 20       | 1.06          |
| (1,496) | 1:19:A:LEU:HD22 | 1:22:A:ASP:HB3  | 20       | 1.06          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,496) | 1:19:A:LEU:HD23 | 1:22:A:ASP:HB3  | 20       | 1.06          |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD11 | 9        | 1.06          |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD12 | 9        | 1.06          |
| (1,480) | 1:13:A:TYR:HB2  | 1:19:A:LEU:HD13 | 9        | 1.06          |
| (1,186) | 1:14:A:LYS:HA   | 1:14:A:LYS:HD2  | 8        | 1.06          |
| (1,186) | 1:14:A:LYS:HA   | 1:14:A:LYS:HD2  | 10       | 1.06          |
| (1,186) | 1:14:A:LYS:HA   | 1:14:A:LYS:HD2  | 19       | 1.06          |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD11 | 14       | 1.05          |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD12 | 14       | 1.05          |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD13 | 14       | 1.05          |
| (1,282) | 1:25:A:SER:HB2  | 1:52:A:ALA:H    | 11       | 1.05          |
| (1,162) | 1:32:A:GLY:HA3  | 1:49:A:ALA:HA   | 8        | 1.05          |
| (1,282) | 1:25:A:SER:HB2  | 1:52:A:ALA:H    | 6        | 1.04          |
| (1,162) | 1:32:A:GLY:HA3  | 1:49:A:ALA:HA   | 2        | 1.04          |
| (1,162) | 1:32:A:GLY:HA3  | 1:49:A:ALA:HA   | 16       | 1.04          |
| (1,354) | 1:16:A:ASP:HB2  | 1:19:A:LEU:HD11 | 1        | 1.03          |
| (1,354) | 1:16:A:ASP:HB2  | 1:19:A:LEU:HD12 | 1        | 1.03          |
| (1,354) | 1:16:A:ASP:HB2  | 1:19:A:LEU:HD13 | 1        | 1.03          |
| (1,262) | 1:21:A:TRP:HA   | 1:24:A:CYS:HB2  | 1        | 1.03          |
| (1,186) | 1:14:A:LYS:HA   | 1:14:A:LYS:HD2  | 7        | 1.03          |
| (1,186) | 1:14:A:LYS:HA   | 1:14:A:LYS:HD2  | 17       | 1.03          |
| (1,162) | 1:32:A:GLY:HA3  | 1:49:A:ALA:HA   | 3        | 1.03          |
| (1,583) | 1:36:A:CYS:HB2  | 1:45:A:SER:HA   | 10       | 1.02          |
| (1,281) | 1:12:A:PRO:HD3  | 1:13:A:TYR:HE1  | 9        | 1.02          |
| (1,281) | 1:12:A:PRO:HD3  | 1:13:A:TYR:HE2  | 9        | 1.02          |
| (1,266) | 1:27:A:GLY:HA3  | 1:53:A:ASP:HA   | 3        | 1.02          |
| (1,251) | 1:26:A:GLY:HA2  | 1:28:A:THR:H    | 12       | 1.02          |
| (1,14)  | 1:14:A:LYS:HD2  | 1:15:A:ASN:H    | 10       | 1.02          |
| (1,583) | 1:36:A:CYS:HB2  | 1:45:A:SER:HA   | 5        | 1.01          |
| (1,496) | 1:19:A:LEU:HD21 | 1:22:A:ASP:HB3  | 12       | 1.01          |
| (1,496) | 1:19:A:LEU:HD22 | 1:22:A:ASP:HB3  | 12       | 1.01          |
| (1,496) | 1:19:A:LEU:HD23 | 1:22:A:ASP:HB3  | 12       | 1.01          |
| (1,482) | 1:7:A:THR:HG21  | 1:41:A:SER:HB3  | 12       | 1.01          |
| (1,482) | 1:7:A:THR:HG22  | 1:41:A:SER:HB3  | 12       | 1.01          |
| (1,482) | 1:7:A:THR:HG23  | 1:41:A:SER:HB3  | 12       | 1.01          |
| (1,162) | 1:32:A:GLY:HA3  | 1:49:A:ALA:HA   | 1        | 1.01          |
| (1,583) | 1:36:A:CYS:HB2  | 1:45:A:SER:HA   | 20       | 1.0           |
| (1,262) | 1:21:A:TRP:HA   | 1:24:A:CYS:HB2  | 20       | 1.0           |
| (1,14)  | 1:14:A:LYS:HD2  | 1:15:A:ASN:H    | 8        | 1.0           |
| (1,282) | 1:25:A:SER:HB2  | 1:52:A:ALA:H    | 12       | 0.99          |
| (1,266) | 1:27:A:GLY:HA3  | 1:53:A:ASP:HA   | 11       | 0.99          |
| (1,251) | 1:26:A:GLY:HA2  | 1:28:A:THR:H    | 19       | 0.99          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,583) | 1:36:A:CYS:HB2  | 1:45:A:SER:HA   | 19       | 0.98          |
| (1,478) | 1:13:A:TYR:HB3  | 1:19:A:LEU:HD11 | 20       | 0.98          |
| (1,478) | 1:13:A:TYR:HB3  | 1:19:A:LEU:HD12 | 20       | 0.98          |
| (1,478) | 1:13:A:TYR:HB3  | 1:19:A:LEU:HD13 | 20       | 0.98          |
| (1,354) | 1:16:A:ASP:HB2  | 1:19:A:LEU:HD11 | 2        | 0.98          |
| (1,354) | 1:16:A:ASP:HB2  | 1:19:A:LEU:HD12 | 2        | 0.98          |
| (1,354) | 1:16:A:ASP:HB2  | 1:19:A:LEU:HD13 | 2        | 0.98          |
| (1,583) | 1:36:A:CYS:HB2  | 1:45:A:SER:HA   | 9        | 0.97          |
| (1,583) | 1:36:A:CYS:HB2  | 1:45:A:SER:HA   | 12       | 0.97          |
| (1,482) | 1:7:A:THR:HG21  | 1:41:A:SER:HB3  | 4        | 0.97          |
| (1,482) | 1:7:A:THR:HG22  | 1:41:A:SER:HB3  | 4        | 0.97          |
| (1,482) | 1:7:A:THR:HG23  | 1:41:A:SER:HB3  | 4        | 0.97          |
| (1,354) | 1:16:A:ASP:HB2  | 1:19:A:LEU:HD11 | 13       | 0.97          |
| (1,354) | 1:16:A:ASP:HB2  | 1:19:A:LEU:HD12 | 13       | 0.97          |
| (1,354) | 1:16:A:ASP:HB2  | 1:19:A:LEU:HD13 | 13       | 0.97          |
| (1,354) | 1:16:A:ASP:HB2  | 1:19:A:LEU:HD11 | 17       | 0.97          |
| (1,354) | 1:16:A:ASP:HB2  | 1:19:A:LEU:HD12 | 17       | 0.97          |
| (1,354) | 1:16:A:ASP:HB2  | 1:19:A:LEU:HD13 | 17       | 0.97          |
| (1,282) | 1:25:A:SER:HB2  | 1:52:A:ALA:H    | 18       | 0.97          |
| (1,583) | 1:36:A:CYS:HB2  | 1:45:A:SER:HA   | 4        | 0.96          |
| (1,583) | 1:36:A:CYS:HB2  | 1:45:A:SER:HA   | 8        | 0.96          |
| (1,583) | 1:36:A:CYS:HB2  | 1:45:A:SER:HA   | 13       | 0.96          |
| (1,583) | 1:36:A:CYS:HB2  | 1:45:A:SER:HA   | 16       | 0.96          |
| (1,482) | 1:7:A:THR:HG21  | 1:41:A:SER:HB3  | 13       | 0.96          |
| (1,482) | 1:7:A:THR:HG22  | 1:41:A:SER:HB3  | 13       | 0.96          |
| (1,482) | 1:7:A:THR:HG23  | 1:41:A:SER:HB3  | 13       | 0.96          |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD11 | 20       | 0.96          |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD12 | 20       | 0.96          |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD13 | 20       | 0.96          |
| (1,14)  | 1:14:A:LYS:HD2  | 1:15:A:ASN:H    | 11       | 0.96          |
| (1,583) | 1:36:A:CYS:HB2  | 1:45:A:SER:HA   | 6        | 0.95          |
| (1,583) | 1:36:A:CYS:HB2  | 1:45:A:SER:HA   | 17       | 0.95          |
| (1,496) | 1:19:A:LEU:HD21 | 1:22:A:ASP:HB3  | 6        | 0.95          |
| (1,496) | 1:19:A:LEU:HD22 | 1:22:A:ASP:HB3  | 6        | 0.95          |
| (1,496) | 1:19:A:LEU:HD23 | 1:22:A:ASP:HB3  | 6        | 0.95          |
| (1,384) | 1:12:A:PRO:HD2  | 1:38:A:GLN:HG2  | 20       | 0.95          |
| (1,384) | 1:12:A:PRO:HD2  | 1:38:A:GLN:HG3  | 20       | 0.95          |
| (1,266) | 1:27:A:GLY:HA3  | 1:53:A:ASP:HA   | 9        | 0.94          |
| (1,266) | 1:27:A:GLY:HA3  | 1:53:A:ASP:HA   | 18       | 0.94          |
| (1,251) | 1:26:A:GLY:HA2  | 1:28:A:THR:H    | 6        | 0.94          |
| (1,482) | 1:7:A:THR:HG21  | 1:41:A:SER:HB3  | 1        | 0.93          |
| (1,482) | 1:7:A:THR:HG22  | 1:41:A:SER:HB3  | 1        | 0.93          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,482) | 1:7:A:THR:HG23  | 1:41:A:SER:HB3  | 1        | 0.93          |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD11 | 11       | 0.93          |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD12 | 11       | 0.93          |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD13 | 11       | 0.93          |
| (1,369) | 1:21:A:TRP:HH2  | 1:51:A:MET:HG2  | 1        | 0.93          |
| (1,197) | 1:27:A:GLY:HA2  | 1:28:A:THR:HG21 | 17       | 0.93          |
| (1,197) | 1:27:A:GLY:HA2  | 1:28:A:THR:HG22 | 17       | 0.93          |
| (1,197) | 1:27:A:GLY:HA2  | 1:28:A:THR:HG23 | 17       | 0.93          |
| (1,266) | 1:27:A:GLY:HA3  | 1:53:A:ASP:HA   | 5        | 0.92          |
| (1,262) | 1:21:A:TRP:HA   | 1:24:A:CYS:HB2  | 3        | 0.92          |
| (1,478) | 1:13:A:TYR:HB3  | 1:19:A:LEU:HD11 | 2        | 0.91          |
| (1,478) | 1:13:A:TYR:HB3  | 1:19:A:LEU:HD12 | 2        | 0.91          |
| (1,478) | 1:13:A:TYR:HB3  | 1:19:A:LEU:HD13 | 2        | 0.91          |
| (1,262) | 1:21:A:TRP:HA   | 1:24:A:CYS:HB2  | 14       | 0.91          |
| (1,354) | 1:16:A:ASP:HB2  | 1:19:A:LEU:HD11 | 6        | 0.9           |
| (1,354) | 1:16:A:ASP:HB2  | 1:19:A:LEU:HD12 | 6        | 0.9           |
| (1,354) | 1:16:A:ASP:HB2  | 1:19:A:LEU:HD13 | 6        | 0.9           |
| (1,197) | 1:27:A:GLY:HA2  | 1:28:A:THR:HG21 | 15       | 0.9           |
| (1,197) | 1:27:A:GLY:HA2  | 1:28:A:THR:HG22 | 15       | 0.9           |
| (1,197) | 1:27:A:GLY:HA2  | 1:28:A:THR:HG23 | 15       | 0.9           |
| (1,482) | 1:7:A:THR:HG21  | 1:41:A:SER:HB3  | 17       | 0.89          |
| (1,482) | 1:7:A:THR:HG22  | 1:41:A:SER:HB3  | 17       | 0.89          |
| (1,482) | 1:7:A:THR:HG23  | 1:41:A:SER:HB3  | 17       | 0.89          |
| (1,496) | 1:19:A:LEU:HD21 | 1:22:A:ASP:HB3  | 14       | 0.88          |
| (1,496) | 1:19:A:LEU:HD22 | 1:22:A:ASP:HB3  | 14       | 0.88          |
| (1,496) | 1:19:A:LEU:HD23 | 1:22:A:ASP:HB3  | 14       | 0.88          |
| (1,197) | 1:27:A:GLY:HA2  | 1:28:A:THR:HG21 | 3        | 0.88          |
| (1,197) | 1:27:A:GLY:HA2  | 1:28:A:THR:HG22 | 3        | 0.88          |
| (1,197) | 1:27:A:GLY:HA2  | 1:28:A:THR:HG23 | 3        | 0.88          |
| (1,482) | 1:7:A:THR:HG21  | 1:41:A:SER:HB3  | 5        | 0.87          |
| (1,482) | 1:7:A:THR:HG22  | 1:41:A:SER:HB3  | 5        | 0.87          |
| (1,482) | 1:7:A:THR:HG23  | 1:41:A:SER:HB3  | 5        | 0.87          |
| (1,478) | 1:13:A:TYR:HB3  | 1:19:A:LEU:HD11 | 4        | 0.87          |
| (1,478) | 1:13:A:TYR:HB3  | 1:19:A:LEU:HD12 | 4        | 0.87          |
| (1,478) | 1:13:A:TYR:HB3  | 1:19:A:LEU:HD13 | 4        | 0.87          |
| (1,162) | 1:32:A:GLY:HA3  | 1:49:A:ALA:HA   | 15       | 0.87          |
| (1,482) | 1:7:A:THR:HG21  | 1:41:A:SER:HB3  | 3        | 0.86          |
| (1,482) | 1:7:A:THR:HG22  | 1:41:A:SER:HB3  | 3        | 0.86          |
| (1,482) | 1:7:A:THR:HG23  | 1:41:A:SER:HB3  | 3        | 0.86          |
| (1,197) | 1:27:A:GLY:HA2  | 1:28:A:THR:HG21 | 10       | 0.86          |
| (1,197) | 1:27:A:GLY:HA2  | 1:28:A:THR:HG22 | 10       | 0.86          |
| (1,197) | 1:27:A:GLY:HA2  | 1:28:A:THR:HG23 | 10       | 0.86          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG21 | 1        | 0.85          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG22 | 1        | 0.85          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG23 | 1        | 0.85          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG21 | 14       | 0.84          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG22 | 14       | 0.84          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG23 | 14       | 0.84          |
| (1,574) | 1:25:A:SER:HB2 | 1:48:A:CYS:HA   | 19       | 0.83          |
| (1,482) | 1:7:A:THR:HG21 | 1:41:A:SER:HB3  | 19       | 0.83          |
| (1,482) | 1:7:A:THR:HG22 | 1:41:A:SER:HB3  | 19       | 0.83          |
| (1,482) | 1:7:A:THR:HG23 | 1:41:A:SER:HB3  | 19       | 0.83          |
| (1,266) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HA   | 13       | 0.83          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG21 | 7        | 0.83          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG22 | 7        | 0.83          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG23 | 7        | 0.83          |
| (1,482) | 1:7:A:THR:HG21 | 1:41:A:SER:HB3  | 6        | 0.82          |
| (1,482) | 1:7:A:THR:HG22 | 1:41:A:SER:HB3  | 6        | 0.82          |
| (1,482) | 1:7:A:THR:HG23 | 1:41:A:SER:HB3  | 6        | 0.82          |
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD11 | 19       | 0.82          |
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD12 | 19       | 0.82          |
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD13 | 19       | 0.82          |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD11 | 19       | 0.82          |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD12 | 19       | 0.82          |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD13 | 19       | 0.82          |
| (1,199) | 1:41:A:SER:HB2 | 1:42:A:PHE:H    | 20       | 0.82          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG21 | 13       | 0.82          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG22 | 13       | 0.82          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG23 | 13       | 0.82          |
| (1,482) | 1:7:A:THR:HG21 | 1:41:A:SER:HB3  | 20       | 0.81          |
| (1,482) | 1:7:A:THR:HG22 | 1:41:A:SER:HB3  | 20       | 0.81          |
| (1,482) | 1:7:A:THR:HG23 | 1:41:A:SER:HB3  | 20       | 0.81          |
| (1,384) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HG2  | 2        | 0.81          |
| (1,384) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HG3  | 2        | 0.81          |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD11 | 14       | 0.81          |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD12 | 14       | 0.81          |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD13 | 14       | 0.81          |
| (1,199) | 1:41:A:SER:HB2 | 1:42:A:PHE:H    | 1        | 0.81          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG21 | 4        | 0.81          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG22 | 4        | 0.81          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG23 | 4        | 0.81          |
| (1,574) | 1:25:A:SER:HB2 | 1:48:A:CYS:HA   | 17       | 0.8           |
| (1,481) | 1:16:A:ASP:HB3 | 1:19:A:LEU:HD11 | 16       | 0.8           |
| (1,481) | 1:16:A:ASP:HB3 | 1:19:A:LEU:HD12 | 16       | 0.8           |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,481) | 1:16:A:ASP:HB3 | 1:19:A:LEU:HD13 | 16       | 0.8           |
| (1,282) | 1:25:A:SER:HB2 | 1:52:A:ALA:H    | 14       | 0.8           |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB2  | 16       | 0.8           |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB3  | 16       | 0.8           |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG21 | 5        | 0.8           |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG22 | 5        | 0.8           |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG23 | 5        | 0.8           |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG21 | 16       | 0.8           |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG22 | 16       | 0.8           |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG23 | 16       | 0.8           |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG21 | 20       | 0.8           |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG22 | 20       | 0.8           |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG23 | 20       | 0.8           |
| (1,384) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HG2  | 1        | 0.79          |
| (1,384) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HG3  | 1        | 0.79          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB2  | 7        | 0.79          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB3  | 7        | 0.79          |
| (1,199) | 1:41:A:SER:HB2 | 1:42:A:PHE:H    | 3        | 0.79          |
| (1,199) | 1:41:A:SER:HB2 | 1:42:A:PHE:H    | 13       | 0.79          |
| (1,199) | 1:41:A:SER:HB2 | 1:42:A:PHE:H    | 19       | 0.79          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG21 | 2        | 0.79          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG22 | 2        | 0.79          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG23 | 2        | 0.79          |
| (1,581) | 1:3:A:GLU:HB2  | 1:17:A:SER:HB2  | 10       | 0.78          |
| (1,574) | 1:25:A:SER:HB2 | 1:48:A:CYS:HA   | 1        | 0.78          |
| (1,511) | 1:2:A:ILE:HG21 | 1:17:A:SER:HB3  | 18       | 0.78          |
| (1,511) | 1:2:A:ILE:HG22 | 1:17:A:SER:HB3  | 18       | 0.78          |
| (1,511) | 1:2:A:ILE:HG23 | 1:17:A:SER:HB3  | 18       | 0.78          |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD11 | 7        | 0.78          |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD12 | 7        | 0.78          |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD13 | 7        | 0.78          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG21 | 8        | 0.78          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG22 | 8        | 0.78          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG23 | 8        | 0.78          |
| (1,282) | 1:25:A:SER:HB2 | 1:52:A:ALA:H    | 1        | 0.77          |
| (1,266) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HA   | 2        | 0.77          |
| (1,199) | 1:41:A:SER:HB2 | 1:42:A:PHE:H    | 6        | 0.77          |
| (1,282) | 1:25:A:SER:HB2 | 1:52:A:ALA:H    | 4        | 0.76          |
| (1,281) | 1:12:A:PRO:HD3 | 1:13:A:TYR:HE1  | 7        | 0.76          |
| (1,281) | 1:12:A:PRO:HD3 | 1:13:A:TYR:HE2  | 7        | 0.76          |
| (1,199) | 1:41:A:SER:HB2 | 1:42:A:PHE:H    | 5        | 0.76          |
| (1,199) | 1:41:A:SER:HB2 | 1:42:A:PHE:H    | 17       | 0.76          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,511) | 1:2:A:ILE:HG21 | 1:17:A:SER:HB3  | 10       | 0.75          |
| (1,511) | 1:2:A:ILE:HG22 | 1:17:A:SER:HB3  | 10       | 0.75          |
| (1,511) | 1:2:A:ILE:HG23 | 1:17:A:SER:HB3  | 10       | 0.75          |
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD11 | 1        | 0.75          |
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD12 | 1        | 0.75          |
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD13 | 1        | 0.75          |
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD11 | 12       | 0.75          |
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD12 | 12       | 0.75          |
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD13 | 12       | 0.75          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB2  | 1        | 0.75          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB3  | 1        | 0.75          |
| (1,199) | 1:41:A:SER:HB2 | 1:42:A:PHE:H    | 4        | 0.75          |
| (1,199) | 1:41:A:SER:HB2 | 1:42:A:PHE:H    | 12       | 0.75          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG21 | 11       | 0.75          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG22 | 11       | 0.75          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG23 | 11       | 0.75          |
| (1,574) | 1:25:A:SER:HB2 | 1:48:A:CYS:HA   | 12       | 0.74          |
| (1,479) | 1:14:A:LYS:HE2 | 1:19:A:LEU:HD11 | 19       | 0.74          |
| (1,479) | 1:14:A:LYS:HE2 | 1:19:A:LEU:HD12 | 19       | 0.74          |
| (1,479) | 1:14:A:LYS:HE2 | 1:19:A:LEU:HD13 | 19       | 0.74          |
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD11 | 11       | 0.74          |
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD12 | 11       | 0.74          |
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD13 | 11       | 0.74          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB2  | 14       | 0.74          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB3  | 14       | 0.74          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG21 | 18       | 0.74          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG22 | 18       | 0.74          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG23 | 18       | 0.74          |
| (1,282) | 1:25:A:SER:HB2 | 1:52:A:ALA:H    | 2        | 0.73          |
| (1,282) | 1:25:A:SER:HB2 | 1:52:A:ALA:H    | 10       | 0.73          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB2  | 3        | 0.73          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB3  | 3        | 0.73          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB2  | 11       | 0.73          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB3  | 11       | 0.73          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB2  | 18       | 0.73          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB3  | 18       | 0.73          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG21 | 9        | 0.73          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG22 | 9        | 0.73          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG23 | 9        | 0.73          |
| (1,511) | 1:2:A:ILE:HG21 | 1:17:A:SER:HB3  | 5        | 0.72          |
| (1,511) | 1:2:A:ILE:HG22 | 1:17:A:SER:HB3  | 5        | 0.72          |
| (1,511) | 1:2:A:ILE:HG23 | 1:17:A:SER:HB3  | 5        | 0.72          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,511) | 1:2:A:ILE:HG21 | 1:17:A:SER:HB3  | 8        | 0.72          |
| (1,511) | 1:2:A:ILE:HG22 | 1:17:A:SER:HB3  | 8        | 0.72          |
| (1,511) | 1:2:A:ILE:HG23 | 1:17:A:SER:HB3  | 8        | 0.72          |
| (1,480) | 1:13:A:TYR:HB2 | 1:19:A:LEU:HD11 | 16       | 0.72          |
| (1,480) | 1:13:A:TYR:HB2 | 1:19:A:LEU:HD12 | 16       | 0.72          |
| (1,480) | 1:13:A:TYR:HB2 | 1:19:A:LEU:HD13 | 16       | 0.72          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB2  | 2        | 0.72          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB3  | 2        | 0.72          |
| (1,94)  | 1:46:A:GLN:HG3 | 1:47:A:SER:H    | 16       | 0.72          |
| (1,511) | 1:2:A:ILE:HG21 | 1:17:A:SER:HB3  | 15       | 0.71          |
| (1,511) | 1:2:A:ILE:HG22 | 1:17:A:SER:HB3  | 15       | 0.71          |
| (1,511) | 1:2:A:ILE:HG23 | 1:17:A:SER:HB3  | 15       | 0.71          |
| (1,282) | 1:25:A:SER:HB2 | 1:52:A:ALA:H    | 13       | 0.71          |
| (1,282) | 1:25:A:SER:HB2 | 1:52:A:ALA:H    | 15       | 0.71          |
| (1,282) | 1:25:A:SER:HB2 | 1:52:A:ALA:H    | 16       | 0.71          |
| (1,266) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HA   | 16       | 0.71          |
| (1,266) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HA   | 17       | 0.71          |
| (1,481) | 1:16:A:ASP:HB3 | 1:19:A:LEU:HD11 | 17       | 0.7           |
| (1,481) | 1:16:A:ASP:HB3 | 1:19:A:LEU:HD12 | 17       | 0.7           |
| (1,481) | 1:16:A:ASP:HB3 | 1:19:A:LEU:HD13 | 17       | 0.7           |
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD11 | 13       | 0.7           |
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD12 | 13       | 0.7           |
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD13 | 13       | 0.7           |
| (1,477) | 1:13:A:TYR:HD1 | 1:19:A:LEU:HD11 | 7        | 0.7           |
| (1,477) | 1:13:A:TYR:HD1 | 1:19:A:LEU:HD12 | 7        | 0.7           |
| (1,477) | 1:13:A:TYR:HD1 | 1:19:A:LEU:HD13 | 7        | 0.7           |
| (1,477) | 1:13:A:TYR:HD2 | 1:19:A:LEU:HD11 | 7        | 0.7           |
| (1,477) | 1:13:A:TYR:HD2 | 1:19:A:LEU:HD12 | 7        | 0.7           |
| (1,477) | 1:13:A:TYR:HD2 | 1:19:A:LEU:HD13 | 7        | 0.7           |
| (1,282) | 1:25:A:SER:HB2 | 1:52:A:ALA:H    | 9        | 0.7           |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG21 | 6        | 0.7           |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG22 | 6        | 0.7           |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG23 | 6        | 0.7           |
| (1,94)  | 1:46:A:GLN:HG3 | 1:47:A:SER:H    | 6        | 0.7           |
| (1,94)  | 1:46:A:GLN:HG3 | 1:47:A:SER:H    | 12       | 0.7           |
| (1,511) | 1:2:A:ILE:HG21 | 1:17:A:SER:HB3  | 12       | 0.69          |
| (1,511) | 1:2:A:ILE:HG22 | 1:17:A:SER:HB3  | 12       | 0.69          |
| (1,511) | 1:2:A:ILE:HG23 | 1:17:A:SER:HB3  | 12       | 0.69          |
| (1,360) | 1:22:A:ASP:HB2 | 1:23:A:THR:H    | 4        | 0.69          |
| (1,581) | 1:3:A:GLU:HB2  | 1:17:A:SER:HB2  | 8        | 0.68          |
| (1,574) | 1:25:A:SER:HB2 | 1:48:A:CYS:HA   | 4        | 0.68          |
| (1,574) | 1:25:A:SER:HB2 | 1:48:A:CYS:HA   | 11       | 0.68          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,511) | 1:2:A:ILE:HG21  | 1:17:A:SER:HB3  | 3        | 0.68          |
| (1,511) | 1:2:A:ILE:HG22  | 1:17:A:SER:HB3  | 3        | 0.68          |
| (1,511) | 1:2:A:ILE:HG23  | 1:17:A:SER:HB3  | 3        | 0.68          |
| (1,496) | 1:19:A:LEU:HD21 | 1:22:A:ASP:HB3  | 19       | 0.68          |
| (1,496) | 1:19:A:LEU:HD22 | 1:22:A:ASP:HB3  | 19       | 0.68          |
| (1,496) | 1:19:A:LEU:HD23 | 1:22:A:ASP:HB3  | 19       | 0.68          |
| (1,282) | 1:25:A:SER:HB2  | 1:52:A:ALA:H    | 7        | 0.68          |
| (1,282) | 1:25:A:SER:HB2  | 1:52:A:ALA:H    | 20       | 0.68          |
| (1,94)  | 1:46:A:GLN:HG3  | 1:47:A:SER:H    | 14       | 0.68          |
| (1,574) | 1:25:A:SER:HB2  | 1:48:A:CYS:HA   | 18       | 0.67          |
| (1,281) | 1:12:A:PRO:HD3  | 1:13:A:TYR:HE1  | 2        | 0.67          |
| (1,281) | 1:12:A:PRO:HD3  | 1:13:A:TYR:HE2  | 2        | 0.67          |
| (1,266) | 1:27:A:GLY:HA3  | 1:53:A:ASP:HA   | 20       | 0.67          |
| (1,605) | 1:27:A:GLY:HA3  | 1:53:A:ASP:HB2  | 8        | 0.66          |
| (1,605) | 1:27:A:GLY:HA3  | 1:53:A:ASP:HB3  | 8        | 0.66          |
| (1,574) | 1:25:A:SER:HB2  | 1:48:A:CYS:HA   | 6        | 0.66          |
| (1,574) | 1:25:A:SER:HB2  | 1:48:A:CYS:HA   | 9        | 0.66          |
| (1,574) | 1:25:A:SER:HB2  | 1:48:A:CYS:HA   | 14       | 0.66          |
| (1,282) | 1:25:A:SER:HB2  | 1:52:A:ALA:H    | 8        | 0.66          |
| (1,251) | 1:26:A:GLY:HA2  | 1:28:A:THR:H    | 11       | 0.66          |
| (1,233) | 1:37:A:GLY:HA3  | 1:45:A:SER:HB2  | 15       | 0.66          |
| (1,233) | 1:37:A:GLY:HA3  | 1:45:A:SER:HB3  | 15       | 0.66          |
| (1,574) | 1:25:A:SER:HB2  | 1:48:A:CYS:HA   | 16       | 0.65          |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD11 | 12       | 0.65          |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD12 | 12       | 0.65          |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD13 | 12       | 0.65          |
| (1,360) | 1:22:A:ASP:HB2  | 1:23:A:THR:H    | 14       | 0.65          |
| (1,281) | 1:12:A:PRO:HD3  | 1:13:A:TYR:HE1  | 17       | 0.65          |
| (1,281) | 1:12:A:PRO:HD3  | 1:13:A:TYR:HE2  | 17       | 0.65          |
| (1,377) | 1:4:A:ASP:HB2   | 1:5:A:PHE:HE1   | 2        | 0.64          |
| (1,377) | 1:4:A:ASP:HB2   | 1:5:A:PHE:HE2   | 2        | 0.64          |
| (1,377) | 1:4:A:ASP:HB2   | 1:5:A:PHE:HE1   | 5        | 0.64          |
| (1,377) | 1:4:A:ASP:HB2   | 1:5:A:PHE:HE2   | 5        | 0.64          |
| (1,377) | 1:4:A:ASP:HB2   | 1:5:A:PHE:HE1   | 11       | 0.64          |
| (1,377) | 1:4:A:ASP:HB2   | 1:5:A:PHE:HE2   | 11       | 0.64          |
| (1,373) | 1:12:A:PRO:HD2  | 1:38:A:GLN:HB2  | 6        | 0.64          |
| (1,373) | 1:12:A:PRO:HD2  | 1:38:A:GLN:HB3  | 6        | 0.64          |
| (1,282) | 1:25:A:SER:HB2  | 1:52:A:ALA:H    | 5        | 0.64          |
| (1,541) | 1:6:A:TYR:HA    | 1:17:A:SER:HB2  | 8        | 0.63          |
| (1,377) | 1:4:A:ASP:HB2   | 1:5:A:PHE:HE1   | 8        | 0.63          |
| (1,377) | 1:4:A:ASP:HB2   | 1:5:A:PHE:HE2   | 8        | 0.63          |
| (1,377) | 1:4:A:ASP:HB2   | 1:5:A:PHE:HE1   | 17       | 0.63          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,377) | 1:4:A:ASP:HB2  | 1:5:A:PHE:HE2   | 17       | 0.63          |
| (1,377) | 1:4:A:ASP:HB2  | 1:5:A:PHE:HE1   | 19       | 0.63          |
| (1,377) | 1:4:A:ASP:HB2  | 1:5:A:PHE:HE2   | 19       | 0.63          |
| (1,377) | 1:4:A:ASP:HB2  | 1:5:A:PHE:HE1   | 20       | 0.63          |
| (1,377) | 1:4:A:ASP:HB2  | 1:5:A:PHE:HE2   | 20       | 0.63          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG21 | 19       | 0.63          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG22 | 19       | 0.63          |
| (1,197) | 1:27:A:GLY:HA2 | 1:28:A:THR:HG23 | 19       | 0.63          |
| (1,94)  | 1:46:A:GLN:HG3 | 1:47:A:SER:H    | 19       | 0.63          |
| (1,541) | 1:6:A:TYR:HA   | 1:17:A:SER:HB2  | 10       | 0.62          |
| (1,511) | 1:2:A:ILE:HG21 | 1:17:A:SER:HB3  | 2        | 0.62          |
| (1,511) | 1:2:A:ILE:HG22 | 1:17:A:SER:HB3  | 2        | 0.62          |
| (1,511) | 1:2:A:ILE:HG23 | 1:17:A:SER:HB3  | 2        | 0.62          |
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD11 | 14       | 0.62          |
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD12 | 14       | 0.62          |
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD13 | 14       | 0.62          |
| (1,377) | 1:4:A:ASP:HB2  | 1:5:A:PHE:HE1   | 4        | 0.62          |
| (1,377) | 1:4:A:ASP:HB2  | 1:5:A:PHE:HE2   | 4        | 0.62          |
| (1,373) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HB2  | 8        | 0.62          |
| (1,373) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HB3  | 8        | 0.62          |
| (1,360) | 1:22:A:ASP:HB2 | 1:23:A:THR:H    | 12       | 0.62          |
| (1,266) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HA   | 15       | 0.62          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB2  | 8        | 0.62          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB3  | 8        | 0.62          |
| (1,94)  | 1:46:A:GLN:HG3 | 1:47:A:SER:H    | 5        | 0.62          |
| (1,94)  | 1:46:A:GLN:HG3 | 1:47:A:SER:H    | 15       | 0.62          |
| (1,574) | 1:25:A:SER:HB2 | 1:48:A:CYS:HA   | 3        | 0.61          |
| (1,574) | 1:25:A:SER:HB2 | 1:48:A:CYS:HA   | 13       | 0.61          |
| (1,481) | 1:16:A:ASP:HB3 | 1:19:A:LEU:HD11 | 7        | 0.61          |
| (1,481) | 1:16:A:ASP:HB3 | 1:19:A:LEU:HD12 | 7        | 0.61          |
| (1,481) | 1:16:A:ASP:HB3 | 1:19:A:LEU:HD13 | 7        | 0.61          |
| (1,480) | 1:13:A:TYR:HB2 | 1:19:A:LEU:HD11 | 7        | 0.61          |
| (1,480) | 1:13:A:TYR:HB2 | 1:19:A:LEU:HD12 | 7        | 0.61          |
| (1,480) | 1:13:A:TYR:HB2 | 1:19:A:LEU:HD13 | 7        | 0.61          |
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD11 | 6        | 0.61          |
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD12 | 6        | 0.61          |
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD13 | 6        | 0.61          |
| (1,373) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HB2  | 18       | 0.61          |
| (1,373) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HB3  | 18       | 0.61          |
| (1,94)  | 1:46:A:GLN:HG3 | 1:47:A:SER:H    | 18       | 0.61          |
| (1,607) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HB3  | 11       | 0.6           |
| (1,574) | 1:25:A:SER:HB2 | 1:48:A:CYS:HA   | 7        | 0.6           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,574) | 1:25:A:SER:HB2  | 1:48:A:CYS:HA   | 10       | 0.6           |
| (1,496) | 1:19:A:LEU:HD21 | 1:22:A:ASP:HB3  | 4        | 0.6           |
| (1,496) | 1:19:A:LEU:HD22 | 1:22:A:ASP:HB3  | 4        | 0.6           |
| (1,496) | 1:19:A:LEU:HD23 | 1:22:A:ASP:HB3  | 4        | 0.6           |
| (1,477) | 1:13:A:TYR:HD1  | 1:19:A:LEU:HD11 | 17       | 0.6           |
| (1,477) | 1:13:A:TYR:HD1  | 1:19:A:LEU:HD12 | 17       | 0.6           |
| (1,477) | 1:13:A:TYR:HD1  | 1:19:A:LEU:HD13 | 17       | 0.6           |
| (1,477) | 1:13:A:TYR:HD2  | 1:19:A:LEU:HD11 | 17       | 0.6           |
| (1,477) | 1:13:A:TYR:HD2  | 1:19:A:LEU:HD12 | 17       | 0.6           |
| (1,477) | 1:13:A:TYR:HD2  | 1:19:A:LEU:HD13 | 17       | 0.6           |
| (1,373) | 1:12:A:PRO:HD2  | 1:38:A:GLN:HB2  | 10       | 0.6           |
| (1,373) | 1:12:A:PRO:HD2  | 1:38:A:GLN:HB3  | 10       | 0.6           |
| (1,373) | 1:12:A:PRO:HD2  | 1:38:A:GLN:HB2  | 19       | 0.6           |
| (1,373) | 1:12:A:PRO:HD2  | 1:38:A:GLN:HB3  | 19       | 0.6           |
| (1,233) | 1:37:A:GLY:HA3  | 1:45:A:SER:HB2  | 4        | 0.6           |
| (1,233) | 1:37:A:GLY:HA3  | 1:45:A:SER:HB3  | 4        | 0.6           |
| (1,94)  | 1:46:A:GLN:HG3  | 1:47:A:SER:H    | 10       | 0.6           |
| (1,605) | 1:27:A:GLY:HA3  | 1:53:A:ASP:HB2  | 19       | 0.59          |
| (1,605) | 1:27:A:GLY:HA3  | 1:53:A:ASP:HB3  | 19       | 0.59          |
| (1,281) | 1:12:A:PRO:HD3  | 1:13:A:TYR:HE1  | 13       | 0.59          |
| (1,281) | 1:12:A:PRO:HD3  | 1:13:A:TYR:HE2  | 13       | 0.59          |
| (1,233) | 1:37:A:GLY:HA3  | 1:45:A:SER:HB2  | 5        | 0.59          |
| (1,233) | 1:37:A:GLY:HA3  | 1:45:A:SER:HB3  | 5        | 0.59          |
| (1,94)  | 1:46:A:GLN:HG3  | 1:47:A:SER:H    | 11       | 0.59          |
| (1,511) | 1:2:A:ILE:HG21  | 1:17:A:SER:HB3  | 11       | 0.58          |
| (1,511) | 1:2:A:ILE:HG22  | 1:17:A:SER:HB3  | 11       | 0.58          |
| (1,511) | 1:2:A:ILE:HG23  | 1:17:A:SER:HB3  | 11       | 0.58          |
| (1,511) | 1:2:A:ILE:HG21  | 1:17:A:SER:HB3  | 14       | 0.58          |
| (1,511) | 1:2:A:ILE:HG22  | 1:17:A:SER:HB3  | 14       | 0.58          |
| (1,511) | 1:2:A:ILE:HG23  | 1:17:A:SER:HB3  | 14       | 0.58          |
| (1,373) | 1:12:A:PRO:HD2  | 1:38:A:GLN:HB2  | 20       | 0.58          |
| (1,373) | 1:12:A:PRO:HD2  | 1:38:A:GLN:HB3  | 20       | 0.58          |
| (1,281) | 1:12:A:PRO:HD3  | 1:13:A:TYR:HE1  | 6        | 0.58          |
| (1,281) | 1:12:A:PRO:HD3  | 1:13:A:TYR:HE2  | 6        | 0.58          |
| (1,197) | 1:27:A:GLY:HA2  | 1:28:A:THR:HG21 | 12       | 0.58          |
| (1,197) | 1:27:A:GLY:HA2  | 1:28:A:THR:HG22 | 12       | 0.58          |
| (1,197) | 1:27:A:GLY:HA2  | 1:28:A:THR:HG23 | 12       | 0.58          |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD11 | 16       | 0.57          |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD12 | 16       | 0.57          |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD13 | 16       | 0.57          |
| (1,373) | 1:12:A:PRO:HD2  | 1:38:A:GLN:HB2  | 3        | 0.57          |
| (1,373) | 1:12:A:PRO:HD2  | 1:38:A:GLN:HB3  | 3        | 0.57          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,373) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HB2  | 5        | 0.57          |
| (1,373) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HB3  | 5        | 0.57          |
| (1,282) | 1:25:A:SER:HB2 | 1:52:A:ALA:H    | 3        | 0.57          |
| (1,605) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HB2  | 5        | 0.56          |
| (1,605) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HB3  | 5        | 0.56          |
| (1,480) | 1:13:A:TYR:HB2 | 1:19:A:LEU:HD11 | 17       | 0.56          |
| (1,480) | 1:13:A:TYR:HB2 | 1:19:A:LEU:HD12 | 17       | 0.56          |
| (1,480) | 1:13:A:TYR:HB2 | 1:19:A:LEU:HD13 | 17       | 0.56          |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD11 | 20       | 0.56          |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD12 | 20       | 0.56          |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD13 | 20       | 0.56          |
| (1,281) | 1:12:A:PRO:HD3 | 1:13:A:TYR:HE1  | 4        | 0.56          |
| (1,281) | 1:12:A:PRO:HD3 | 1:13:A:TYR:HE2  | 4        | 0.56          |
| (1,266) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HA   | 7        | 0.56          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB2  | 9        | 0.56          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB3  | 9        | 0.56          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB2  | 10       | 0.56          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB3  | 10       | 0.56          |
| (1,360) | 1:22:A:ASP:HB2 | 1:23:A:THR:H    | 19       | 0.55          |
| (1,251) | 1:26:A:GLY:HA2 | 1:28:A:THR:H    | 18       | 0.55          |
| (1,607) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HB3  | 9        | 0.54          |
| (1,511) | 1:2:A:ILE:HG21 | 1:17:A:SER:HB3  | 9        | 0.54          |
| (1,511) | 1:2:A:ILE:HG22 | 1:17:A:SER:HB3  | 9        | 0.54          |
| (1,511) | 1:2:A:ILE:HG23 | 1:17:A:SER:HB3  | 9        | 0.54          |
| (1,360) | 1:22:A:ASP:HB2 | 1:23:A:THR:H    | 15       | 0.54          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB2  | 17       | 0.54          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB3  | 17       | 0.54          |
| (1,574) | 1:25:A:SER:HB2 | 1:48:A:CYS:HA   | 2        | 0.53          |
| (1,384) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HG2  | 12       | 0.53          |
| (1,384) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HG3  | 12       | 0.53          |
| (1,320) | 1:36:A:CYS:H   | 1:36:A:CYS:HB3  | 4        | 0.52          |
| (1,320) | 1:36:A:CYS:H   | 1:36:A:CYS:HB3  | 5        | 0.52          |
| (1,320) | 1:36:A:CYS:H   | 1:36:A:CYS:HB3  | 6        | 0.52          |
| (1,320) | 1:36:A:CYS:H   | 1:36:A:CYS:HB3  | 8        | 0.52          |
| (1,320) | 1:36:A:CYS:H   | 1:36:A:CYS:HB3  | 9        | 0.52          |
| (1,320) | 1:36:A:CYS:H   | 1:36:A:CYS:HB3  | 10       | 0.52          |
| (1,320) | 1:36:A:CYS:H   | 1:36:A:CYS:HB3  | 12       | 0.52          |
| (1,320) | 1:36:A:CYS:H   | 1:36:A:CYS:HB3  | 13       | 0.52          |
| (1,320) | 1:36:A:CYS:H   | 1:36:A:CYS:HB3  | 16       | 0.52          |
| (1,320) | 1:36:A:CYS:H   | 1:36:A:CYS:HB3  | 17       | 0.52          |
| (1,320) | 1:36:A:CYS:H   | 1:36:A:CYS:HB3  | 19       | 0.52          |
| (1,320) | 1:36:A:CYS:H   | 1:36:A:CYS:HB3  | 20       | 0.52          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,574) | 1:25:A:SER:HB2 | 1:48:A:CYS:HA   | 20       | 0.51          |
| (1,536) | 1:21:A:TRP:HZ3 | 1:25:A:SER:HB2  | 17       | 0.51          |
| (1,511) | 1:2:A:ILE:HG21 | 1:17:A:SER:HB3  | 1        | 0.51          |
| (1,511) | 1:2:A:ILE:HG22 | 1:17:A:SER:HB3  | 1        | 0.51          |
| (1,511) | 1:2:A:ILE:HG23 | 1:17:A:SER:HB3  | 1        | 0.51          |
| (1,511) | 1:2:A:ILE:HG21 | 1:17:A:SER:HB3  | 19       | 0.51          |
| (1,511) | 1:2:A:ILE:HG22 | 1:17:A:SER:HB3  | 19       | 0.51          |
| (1,511) | 1:2:A:ILE:HG23 | 1:17:A:SER:HB3  | 19       | 0.51          |
| (1,373) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HB2  | 2        | 0.51          |
| (1,373) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HB3  | 2        | 0.51          |
| (1,605) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HB2  | 6        | 0.5           |
| (1,605) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HB3  | 6        | 0.5           |
| (1,605) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HB2  | 12       | 0.5           |
| (1,605) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HB3  | 12       | 0.5           |
| (1,581) | 1:3:A:GLU:HB2  | 1:17:A:SER:HB2  | 20       | 0.5           |
| (1,511) | 1:2:A:ILE:HG21 | 1:17:A:SER:HB3  | 4        | 0.5           |
| (1,511) | 1:2:A:ILE:HG22 | 1:17:A:SER:HB3  | 4        | 0.5           |
| (1,511) | 1:2:A:ILE:HG23 | 1:17:A:SER:HB3  | 4        | 0.5           |
| (1,511) | 1:2:A:ILE:HG21 | 1:17:A:SER:HB3  | 16       | 0.5           |
| (1,511) | 1:2:A:ILE:HG22 | 1:17:A:SER:HB3  | 16       | 0.5           |
| (1,511) | 1:2:A:ILE:HG23 | 1:17:A:SER:HB3  | 16       | 0.5           |
| (1,477) | 1:13:A:TYR:HD1 | 1:19:A:LEU:HD11 | 11       | 0.5           |
| (1,477) | 1:13:A:TYR:HD1 | 1:19:A:LEU:HD12 | 11       | 0.5           |
| (1,477) | 1:13:A:TYR:HD1 | 1:19:A:LEU:HD13 | 11       | 0.5           |
| (1,477) | 1:13:A:TYR:HD2 | 1:19:A:LEU:HD11 | 11       | 0.5           |
| (1,477) | 1:13:A:TYR:HD2 | 1:19:A:LEU:HD12 | 11       | 0.5           |
| (1,477) | 1:13:A:TYR:HD2 | 1:19:A:LEU:HD13 | 11       | 0.5           |
| (1,384) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HG2  | 11       | 0.5           |
| (1,384) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HG3  | 11       | 0.5           |
| (1,373) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HB2  | 11       | 0.5           |
| (1,373) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HB3  | 11       | 0.5           |
| (1,373) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HB2  | 14       | 0.5           |
| (1,373) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HB3  | 14       | 0.5           |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD11 | 4        | 0.5           |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD12 | 4        | 0.5           |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD13 | 4        | 0.5           |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD11 | 5        | 0.5           |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD12 | 5        | 0.5           |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD13 | 5        | 0.5           |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD11 | 15       | 0.5           |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD12 | 15       | 0.5           |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD13 | 15       | 0.5           |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD11 | 18       | 0.5           |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD12 | 18       | 0.5           |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD13 | 18       | 0.5           |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB2  | 13       | 0.5           |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB3  | 13       | 0.5           |
| (1,94)  | 1:46:A:GLN:HG3 | 1:47:A:SER:H    | 3        | 0.5           |
| (1,511) | 1:2:A:ILE:HG21 | 1:17:A:SER:HB3  | 6        | 0.49          |
| (1,511) | 1:2:A:ILE:HG22 | 1:17:A:SER:HB3  | 6        | 0.49          |
| (1,511) | 1:2:A:ILE:HG23 | 1:17:A:SER:HB3  | 6        | 0.49          |
| (1,373) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HB2  | 7        | 0.49          |
| (1,373) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HB3  | 7        | 0.49          |
| (1,266) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HA   | 4        | 0.49          |
| (1,579) | 1:6:A:TYR:HD1  | 1:17:A:SER:HB2  | 2        | 0.48          |
| (1,579) | 1:6:A:TYR:HD2  | 1:17:A:SER:HB2  | 2        | 0.48          |
| (1,574) | 1:25:A:SER:HB2 | 1:48:A:CYS:HA   | 15       | 0.48          |
| (1,384) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HG2  | 4        | 0.48          |
| (1,384) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HG3  | 4        | 0.48          |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD11 | 3        | 0.48          |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD12 | 3        | 0.48          |
| (1,354) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HD13 | 3        | 0.48          |
| (1,581) | 1:3:A:GLU:HB2  | 1:17:A:SER:HB2  | 1        | 0.47          |
| (1,373) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HB2  | 1        | 0.47          |
| (1,373) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HB3  | 1        | 0.47          |
| (1,266) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HA   | 1        | 0.47          |
| (1,605) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HB2  | 16       | 0.46          |
| (1,605) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HB3  | 16       | 0.46          |
| (1,436) | 1:14:A:LYS:HB2 | 1:14:A:LYS:HD2  | 18       | 0.46          |
| (1,436) | 1:14:A:LYS:HB3 | 1:14:A:LYS:HD2  | 18       | 0.46          |
| (1,436) | 1:14:A:LYS:HB2 | 1:14:A:LYS:HD2  | 20       | 0.46          |
| (1,436) | 1:14:A:LYS:HB3 | 1:14:A:LYS:HD2  | 20       | 0.46          |
| (1,281) | 1:12:A:PRO:HD3 | 1:13:A:TYR:HE1  | 12       | 0.46          |
| (1,281) | 1:12:A:PRO:HD3 | 1:13:A:TYR:HE2  | 12       | 0.46          |
| (1,243) | 1:11:A:CYS:H   | 1:12:A:PRO:HD2  | 1        | 0.46          |
| (1,243) | 1:11:A:CYS:H   | 1:12:A:PRO:HD2  | 2        | 0.46          |
| (1,243) | 1:11:A:CYS:H   | 1:12:A:PRO:HD2  | 3        | 0.46          |
| (1,243) | 1:11:A:CYS:H   | 1:12:A:PRO:HD2  | 4        | 0.46          |
| (1,243) | 1:11:A:CYS:H   | 1:12:A:PRO:HD2  | 5        | 0.46          |
| (1,243) | 1:11:A:CYS:H   | 1:12:A:PRO:HD2  | 6        | 0.46          |
| (1,243) | 1:11:A:CYS:H   | 1:12:A:PRO:HD2  | 7        | 0.46          |
| (1,243) | 1:11:A:CYS:H   | 1:12:A:PRO:HD2  | 8        | 0.46          |
| (1,243) | 1:11:A:CYS:H   | 1:12:A:PRO:HD2  | 9        | 0.46          |
| (1,243) | 1:11:A:CYS:H   | 1:12:A:PRO:HD2  | 10       | 0.46          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,243) | 1:11:A:CYS:H   | 1:12:A:PRO:HD2 | 11       | 0.46          |
| (1,243) | 1:11:A:CYS:H   | 1:12:A:PRO:HD2 | 12       | 0.46          |
| (1,243) | 1:11:A:CYS:H   | 1:12:A:PRO:HD2 | 13       | 0.46          |
| (1,243) | 1:11:A:CYS:H   | 1:12:A:PRO:HD2 | 14       | 0.46          |
| (1,243) | 1:11:A:CYS:H   | 1:12:A:PRO:HD2 | 15       | 0.46          |
| (1,243) | 1:11:A:CYS:H   | 1:12:A:PRO:HD2 | 16       | 0.46          |
| (1,243) | 1:11:A:CYS:H   | 1:12:A:PRO:HD2 | 17       | 0.46          |
| (1,243) | 1:11:A:CYS:H   | 1:12:A:PRO:HD2 | 18       | 0.46          |
| (1,243) | 1:11:A:CYS:H   | 1:12:A:PRO:HD2 | 19       | 0.46          |
| (1,243) | 1:11:A:CYS:H   | 1:12:A:PRO:HD2 | 20       | 0.46          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB2 | 20       | 0.46          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB3 | 20       | 0.46          |
| (1,607) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HB3 | 14       | 0.45          |
| (1,593) | 1:59:A:ASN:HB2 | 1:60:A:ALA:HB1 | 8        | 0.45          |
| (1,593) | 1:59:A:ASN:HB2 | 1:60:A:ALA:HB2 | 8        | 0.45          |
| (1,593) | 1:59:A:ASN:HB2 | 1:60:A:ALA:HB3 | 8        | 0.45          |
| (1,574) | 1:25:A:SER:HB2 | 1:48:A:CYS:HA  | 5        | 0.45          |
| (1,436) | 1:14:A:LYS:HB2 | 1:14:A:LYS:HD2 | 8        | 0.45          |
| (1,436) | 1:14:A:LYS:HB3 | 1:14:A:LYS:HD2 | 8        | 0.45          |
| (1,436) | 1:14:A:LYS:HB2 | 1:14:A:LYS:HD2 | 10       | 0.45          |
| (1,436) | 1:14:A:LYS:HB3 | 1:14:A:LYS:HD2 | 10       | 0.45          |
| (1,436) | 1:14:A:LYS:HB2 | 1:14:A:LYS:HD2 | 11       | 0.45          |
| (1,436) | 1:14:A:LYS:HB3 | 1:14:A:LYS:HD2 | 11       | 0.45          |
| (1,436) | 1:14:A:LYS:HB2 | 1:14:A:LYS:HD2 | 12       | 0.45          |
| (1,436) | 1:14:A:LYS:HB3 | 1:14:A:LYS:HD2 | 12       | 0.45          |
| (1,436) | 1:14:A:LYS:HB2 | 1:14:A:LYS:HD2 | 19       | 0.45          |
| (1,436) | 1:14:A:LYS:HB3 | 1:14:A:LYS:HD2 | 19       | 0.45          |
| (1,402) | 1:3:A:GLU:H    | 1:3:A:GLU:HB2  | 2        | 0.45          |
| (1,402) | 1:3:A:GLU:H    | 1:3:A:GLU:HB2  | 3        | 0.45          |
| (1,402) | 1:3:A:GLU:H    | 1:3:A:GLU:HB2  | 4        | 0.45          |
| (1,402) | 1:3:A:GLU:H    | 1:3:A:GLU:HB2  | 8        | 0.45          |
| (1,402) | 1:3:A:GLU:H    | 1:3:A:GLU:HB2  | 9        | 0.45          |
| (1,402) | 1:3:A:GLU:H    | 1:3:A:GLU:HB2  | 10       | 0.45          |
| (1,402) | 1:3:A:GLU:H    | 1:3:A:GLU:HB2  | 11       | 0.45          |
| (1,402) | 1:3:A:GLU:H    | 1:3:A:GLU:HB2  | 12       | 0.45          |
| (1,402) | 1:3:A:GLU:H    | 1:3:A:GLU:HB2  | 14       | 0.45          |
| (1,402) | 1:3:A:GLU:H    | 1:3:A:GLU:HB2  | 16       | 0.45          |
| (1,402) | 1:3:A:GLU:H    | 1:3:A:GLU:HB2  | 18       | 0.45          |
| (1,402) | 1:3:A:GLU:H    | 1:3:A:GLU:HB2  | 19       | 0.45          |
| (1,402) | 1:3:A:GLU:H    | 1:3:A:GLU:HB2  | 20       | 0.45          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB2 | 12       | 0.45          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB3 | 12       | 0.45          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,94)  | 1:46:A:GLN:HG3 | 1:47:A:SER:H    | 2        | 0.45          |
| (1,607) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HB3  | 1        | 0.44          |
| (1,436) | 1:14:A:LYS:HB2 | 1:14:A:LYS:HD2  | 2        | 0.44          |
| (1,436) | 1:14:A:LYS:HB3 | 1:14:A:LYS:HD2  | 2        | 0.44          |
| (1,360) | 1:22:A:ASP:HB2 | 1:23:A:THR:H    | 17       | 0.44          |
| (1,607) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HB3  | 12       | 0.43          |
| (1,605) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HB2  | 13       | 0.43          |
| (1,605) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HB3  | 13       | 0.43          |
| (1,605) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HB2  | 18       | 0.43          |
| (1,605) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HB3  | 18       | 0.43          |
| (1,605) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HB2  | 20       | 0.43          |
| (1,605) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HB3  | 20       | 0.43          |
| (1,574) | 1:25:A:SER:HB2 | 1:48:A:CYS:HA   | 8        | 0.43          |
| (1,373) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HB2  | 15       | 0.43          |
| (1,373) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HB3  | 15       | 0.43          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB2  | 6        | 0.43          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB3  | 6        | 0.43          |
| (1,581) | 1:3:A:GLU:HB2  | 1:17:A:SER:HB2  | 6        | 0.42          |
| (1,579) | 1:6:A:TYR:HD1  | 1:17:A:SER:HB2  | 10       | 0.42          |
| (1,579) | 1:6:A:TYR:HD2  | 1:17:A:SER:HB2  | 10       | 0.42          |
| (1,366) | 1:24:A:CYS:HB3 | 1:35:A:CYS:HB2  | 20       | 0.41          |
| (1,285) | 1:17:A:SER:H   | 1:17:A:SER:HB2  | 16       | 0.41          |
| (1,605) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HB2  | 11       | 0.4           |
| (1,605) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HB3  | 11       | 0.4           |
| (1,373) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HB2  | 12       | 0.4           |
| (1,373) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HB3  | 12       | 0.4           |
| (1,285) | 1:17:A:SER:H   | 1:17:A:SER:HB2  | 9        | 0.4           |
| (1,285) | 1:17:A:SER:H   | 1:17:A:SER:HB2  | 14       | 0.4           |
| (1,285) | 1:17:A:SER:H   | 1:17:A:SER:HB2  | 19       | 0.4           |
| (1,94)  | 1:46:A:GLN:HG3 | 1:47:A:SER:H    | 7        | 0.4           |
| (1,575) | 1:6:A:TYR:HE1  | 1:17:A:SER:HB2  | 2        | 0.39          |
| (1,575) | 1:6:A:TYR:HE2  | 1:17:A:SER:HB2  | 2        | 0.39          |
| (1,541) | 1:6:A:TYR:HA   | 1:17:A:SER:HB2  | 6        | 0.39          |
| (1,477) | 1:13:A:TYR:HD1 | 1:19:A:LEU:HD11 | 19       | 0.39          |
| (1,477) | 1:13:A:TYR:HD1 | 1:19:A:LEU:HD12 | 19       | 0.39          |
| (1,477) | 1:13:A:TYR:HD1 | 1:19:A:LEU:HD13 | 19       | 0.39          |
| (1,477) | 1:13:A:TYR:HD2 | 1:19:A:LEU:HD11 | 19       | 0.39          |
| (1,477) | 1:13:A:TYR:HD2 | 1:19:A:LEU:HD12 | 19       | 0.39          |
| (1,477) | 1:13:A:TYR:HD2 | 1:19:A:LEU:HD13 | 19       | 0.39          |
| (1,360) | 1:22:A:ASP:HB2 | 1:23:A:THR:H    | 5        | 0.39          |
| (1,285) | 1:17:A:SER:H   | 1:17:A:SER:HB2  | 1        | 0.39          |
| (1,285) | 1:17:A:SER:H   | 1:17:A:SER:HB2  | 2        | 0.39          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,285) | 1:17:A:SER:H   | 1:17:A:SER:HB2  | 4        | 0.39          |
| (1,285) | 1:17:A:SER:H   | 1:17:A:SER:HB2  | 18       | 0.39          |
| (1,14)  | 1:14:A:LYS:HD2 | 1:15:A:ASN:H    | 7        | 0.39          |
| (1,14)  | 1:14:A:LYS:HD2 | 1:15:A:ASN:H    | 17       | 0.39          |
| (1,605) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HB2  | 2        | 0.38          |
| (1,605) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HB3  | 2        | 0.38          |
| (1,605) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HB2  | 15       | 0.38          |
| (1,605) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HB3  | 15       | 0.38          |
| (1,436) | 1:14:A:LYS:HB2 | 1:14:A:LYS:HD2  | 17       | 0.38          |
| (1,436) | 1:14:A:LYS:HB3 | 1:14:A:LYS:HD2  | 17       | 0.38          |
| (1,384) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HG2  | 3        | 0.38          |
| (1,384) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HG3  | 3        | 0.38          |
| (1,285) | 1:17:A:SER:H   | 1:17:A:SER:HB2  | 3        | 0.38          |
| (1,285) | 1:17:A:SER:H   | 1:17:A:SER:HB2  | 6        | 0.38          |
| (1,285) | 1:17:A:SER:H   | 1:17:A:SER:HB2  | 11       | 0.38          |
| (1,285) | 1:17:A:SER:H   | 1:17:A:SER:HB2  | 12       | 0.38          |
| (1,45)  | 1:15:A:ASN:HB2 | 1:16:A:ASP:H    | 12       | 0.38          |
| (1,621) | 1:3:A:GLU:HA   | 1:3:A:GLU:HG3   | 4        | 0.37          |
| (1,579) | 1:6:A:TYR:HD1  | 1:17:A:SER:HB2  | 8        | 0.37          |
| (1,579) | 1:6:A:TYR:HD2  | 1:17:A:SER:HB2  | 8        | 0.37          |
| (1,579) | 1:6:A:TYR:HD1  | 1:17:A:SER:HB2  | 11       | 0.37          |
| (1,579) | 1:6:A:TYR:HD2  | 1:17:A:SER:HB2  | 11       | 0.37          |
| (1,481) | 1:16:A:ASP:HB3 | 1:19:A:LEU:HD11 | 4        | 0.37          |
| (1,481) | 1:16:A:ASP:HB3 | 1:19:A:LEU:HD12 | 4        | 0.37          |
| (1,481) | 1:16:A:ASP:HB3 | 1:19:A:LEU:HD13 | 4        | 0.37          |
| (1,436) | 1:14:A:LYS:HB2 | 1:14:A:LYS:HD2  | 7        | 0.37          |
| (1,436) | 1:14:A:LYS:HB3 | 1:14:A:LYS:HD2  | 7        | 0.37          |
| (1,384) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HG2  | 9        | 0.37          |
| (1,384) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HG3  | 9        | 0.37          |
| (1,285) | 1:17:A:SER:H   | 1:17:A:SER:HB2  | 15       | 0.37          |
| (1,281) | 1:12:A:PRO:HD3 | 1:13:A:TYR:HE1  | 19       | 0.37          |
| (1,281) | 1:12:A:PRO:HD3 | 1:13:A:TYR:HE2  | 19       | 0.37          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB2  | 19       | 0.37          |
| (1,233) | 1:37:A:GLY:HA3 | 1:45:A:SER:HB3  | 19       | 0.37          |
| (1,45)  | 1:15:A:ASN:HB2 | 1:16:A:ASP:H    | 13       | 0.37          |
| (1,579) | 1:6:A:TYR:HD1  | 1:17:A:SER:HB2  | 12       | 0.36          |
| (1,579) | 1:6:A:TYR:HD2  | 1:17:A:SER:HB2  | 12       | 0.36          |
| (1,541) | 1:6:A:TYR:HA   | 1:17:A:SER:HB2  | 5        | 0.36          |
| (1,477) | 1:13:A:TYR:HD1 | 1:19:A:LEU:HD11 | 4        | 0.36          |
| (1,477) | 1:13:A:TYR:HD1 | 1:19:A:LEU:HD12 | 4        | 0.36          |
| (1,477) | 1:13:A:TYR:HD1 | 1:19:A:LEU:HD13 | 4        | 0.36          |
| (1,477) | 1:13:A:TYR:HD2 | 1:19:A:LEU:HD11 | 4        | 0.36          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,477) | 1:13:A:TYR:HD2 | 1:19:A:LEU:HD12 | 4        | 0.36          |
| (1,477) | 1:13:A:TYR:HD2 | 1:19:A:LEU:HD13 | 4        | 0.36          |
| (1,285) | 1:17:A:SER:H   | 1:17:A:SER:HB2  | 5        | 0.36          |
| (1,45)  | 1:15:A:ASN:HB2 | 1:16:A:ASP:H    | 11       | 0.36          |
| (1,605) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HB2  | 9        | 0.35          |
| (1,605) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HB3  | 9        | 0.35          |
| (1,104) | 1:44:A:VAL:H   | 1:45:A:SER:HA   | 7        | 0.35          |
| (1,45)  | 1:15:A:ASN:HB2 | 1:16:A:ASP:H    | 14       | 0.35          |
| (1,550) | 1:41:A:SER:HA  | 1:41:A:SER:HB2  | 4        | 0.34          |
| (1,550) | 1:41:A:SER:HA  | 1:41:A:SER:HB2  | 5        | 0.34          |
| (1,550) | 1:41:A:SER:HA  | 1:41:A:SER:HB2  | 6        | 0.34          |
| (1,550) | 1:41:A:SER:HA  | 1:41:A:SER:HB2  | 12       | 0.34          |
| (1,550) | 1:41:A:SER:HA  | 1:41:A:SER:HB2  | 17       | 0.34          |
| (1,550) | 1:41:A:SER:HA  | 1:41:A:SER:HB2  | 19       | 0.34          |
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD11 | 9        | 0.34          |
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD12 | 9        | 0.34          |
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD13 | 9        | 0.34          |
| (1,104) | 1:44:A:VAL:H   | 1:45:A:SER:HA   | 1        | 0.34          |
| (1,104) | 1:44:A:VAL:H   | 1:45:A:SER:HA   | 2        | 0.34          |
| (1,104) | 1:44:A:VAL:H   | 1:45:A:SER:HA   | 5        | 0.34          |
| (1,104) | 1:44:A:VAL:H   | 1:45:A:SER:HA   | 6        | 0.34          |
| (1,104) | 1:44:A:VAL:H   | 1:45:A:SER:HA   | 8        | 0.34          |
| (1,104) | 1:44:A:VAL:H   | 1:45:A:SER:HA   | 9        | 0.34          |
| (1,104) | 1:44:A:VAL:H   | 1:45:A:SER:HA   | 11       | 0.34          |
| (1,104) | 1:44:A:VAL:H   | 1:45:A:SER:HA   | 13       | 0.34          |
| (1,104) | 1:44:A:VAL:H   | 1:45:A:SER:HA   | 15       | 0.34          |
| (1,104) | 1:44:A:VAL:H   | 1:45:A:SER:HA   | 16       | 0.34          |
| (1,104) | 1:44:A:VAL:H   | 1:45:A:SER:HA   | 17       | 0.34          |
| (1,639) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HB2  | 9        | 0.33          |
| (1,639) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HB2  | 11       | 0.33          |
| (1,607) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HB3  | 2        | 0.33          |
| (1,550) | 1:41:A:SER:HA  | 1:41:A:SER:HB2  | 1        | 0.33          |
| (1,550) | 1:41:A:SER:HA  | 1:41:A:SER:HB2  | 3        | 0.33          |
| (1,550) | 1:41:A:SER:HA  | 1:41:A:SER:HB2  | 13       | 0.33          |
| (1,477) | 1:13:A:TYR:HD1 | 1:19:A:LEU:HD11 | 1        | 0.33          |
| (1,477) | 1:13:A:TYR:HD1 | 1:19:A:LEU:HD12 | 1        | 0.33          |
| (1,477) | 1:13:A:TYR:HD1 | 1:19:A:LEU:HD13 | 1        | 0.33          |
| (1,477) | 1:13:A:TYR:HD2 | 1:19:A:LEU:HD11 | 1        | 0.33          |
| (1,477) | 1:13:A:TYR:HD2 | 1:19:A:LEU:HD12 | 1        | 0.33          |
| (1,477) | 1:13:A:TYR:HD2 | 1:19:A:LEU:HD13 | 1        | 0.33          |
| (1,385) | 1:3:A:GLU:H    | 1:3:A:GLU:HG2   | 7        | 0.33          |
| (1,384) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HG2  | 13       | 0.33          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,384) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HG3  | 13       | 0.33          |
| (1,384) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HG2  | 14       | 0.33          |
| (1,384) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HG3  | 14       | 0.33          |
| (1,104) | 1:44:A:VAL:H   | 1:45:A:SER:HA   | 3        | 0.33          |
| (1,104) | 1:44:A:VAL:H   | 1:45:A:SER:HA   | 4        | 0.33          |
| (1,104) | 1:44:A:VAL:H   | 1:45:A:SER:HA   | 10       | 0.33          |
| (1,104) | 1:44:A:VAL:H   | 1:45:A:SER:HA   | 12       | 0.33          |
| (1,104) | 1:44:A:VAL:H   | 1:45:A:SER:HA   | 14       | 0.33          |
| (1,104) | 1:44:A:VAL:H   | 1:45:A:SER:HA   | 18       | 0.33          |
| (1,104) | 1:44:A:VAL:H   | 1:45:A:SER:HA   | 19       | 0.33          |
| (1,639) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HB2  | 12       | 0.32          |
| (1,614) | 1:46:A:GLN:HA  | 1:46:A:GLN:HG2  | 17       | 0.32          |
| (1,385) | 1:3:A:GLU:H    | 1:3:A:GLU:HG2   | 1        | 0.32          |
| (1,385) | 1:3:A:GLU:H    | 1:3:A:GLU:HG2   | 15       | 0.32          |
| (1,104) | 1:44:A:VAL:H   | 1:45:A:SER:HA   | 20       | 0.32          |
| (1,639) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HB2  | 6        | 0.31          |
| (1,618) | 1:3:A:GLU:HB2  | 1:3:A:GLU:HG2   | 19       | 0.31          |
| (1,614) | 1:46:A:GLN:HA  | 1:46:A:GLN:HG2  | 1        | 0.31          |
| (1,550) | 1:41:A:SER:HA  | 1:41:A:SER:HB2  | 20       | 0.31          |
| (1,477) | 1:13:A:TYR:HD1 | 1:19:A:LEU:HD11 | 6        | 0.31          |
| (1,477) | 1:13:A:TYR:HD1 | 1:19:A:LEU:HD12 | 6        | 0.31          |
| (1,477) | 1:13:A:TYR:HD1 | 1:19:A:LEU:HD13 | 6        | 0.31          |
| (1,477) | 1:13:A:TYR:HD2 | 1:19:A:LEU:HD11 | 6        | 0.31          |
| (1,477) | 1:13:A:TYR:HD2 | 1:19:A:LEU:HD12 | 6        | 0.31          |
| (1,477) | 1:13:A:TYR:HD2 | 1:19:A:LEU:HD13 | 6        | 0.31          |
| (1,414) | 1:3:A:GLU:HB3  | 1:4:A:ASP:H     | 20       | 0.31          |
| (1,385) | 1:3:A:GLU:H    | 1:3:A:GLU:HG2   | 5        | 0.31          |
| (1,373) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HB2  | 13       | 0.31          |
| (1,373) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HB3  | 13       | 0.31          |
| (1,285) | 1:17:A:SER:H   | 1:17:A:SER:HB2  | 8        | 0.31          |
| (1,285) | 1:17:A:SER:H   | 1:17:A:SER:HB2  | 10       | 0.31          |
| (1,74)  | 1:16:A:ASP:HB2 | 1:18:A:GLN:H    | 15       | 0.31          |
| (1,618) | 1:3:A:GLU:HB2  | 1:3:A:GLU:HG2   | 8        | 0.3           |
| (1,618) | 1:3:A:GLU:HB2  | 1:3:A:GLU:HG2   | 11       | 0.3           |
| (1,618) | 1:3:A:GLU:HB2  | 1:3:A:GLU:HG2   | 12       | 0.3           |
| (1,614) | 1:46:A:GLN:HA  | 1:46:A:GLN:HG2  | 20       | 0.3           |
| (1,605) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HB2  | 7        | 0.3           |
| (1,605) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HB3  | 7        | 0.3           |
| (1,594) | 1:56:A:ASP:HA  | 1:56:A:ASP:HB2  | 18       | 0.3           |
| (1,384) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HG2  | 17       | 0.3           |
| (1,384) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HG3  | 17       | 0.3           |
| (1,74)  | 1:16:A:ASP:HB2 | 1:18:A:GLN:H    | 14       | 0.3           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,618) | 1:3:A:GLU:HB2   | 1:3:A:GLU:HG2   | 9        | 0.29          |
| (1,614) | 1:46:A:GLN:HA   | 1:46:A:GLN:HG2  | 13       | 0.29          |
| (1,594) | 1:56:A:ASP:HA   | 1:56:A:ASP:HB2  | 1        | 0.29          |
| (1,594) | 1:56:A:ASP:HA   | 1:56:A:ASP:HB2  | 11       | 0.29          |
| (1,594) | 1:56:A:ASP:HA   | 1:56:A:ASP:HB2  | 15       | 0.29          |
| (1,594) | 1:56:A:ASP:HA   | 1:56:A:ASP:HB2  | 19       | 0.29          |
| (1,594) | 1:56:A:ASP:HA   | 1:56:A:ASP:HB2  | 20       | 0.29          |
| (1,536) | 1:21:A:TRP:HZ3  | 1:25:A:SER:HB2  | 3        | 0.29          |
| (1,477) | 1:13:A:TYR:HD1  | 1:19:A:LEU:HD11 | 14       | 0.29          |
| (1,477) | 1:13:A:TYR:HD1  | 1:19:A:LEU:HD12 | 14       | 0.29          |
| (1,477) | 1:13:A:TYR:HD1  | 1:19:A:LEU:HD13 | 14       | 0.29          |
| (1,477) | 1:13:A:TYR:HD2  | 1:19:A:LEU:HD11 | 14       | 0.29          |
| (1,477) | 1:13:A:TYR:HD2  | 1:19:A:LEU:HD12 | 14       | 0.29          |
| (1,477) | 1:13:A:TYR:HD2  | 1:19:A:LEU:HD13 | 14       | 0.29          |
| (1,477) | 1:13:A:TYR:HD1  | 1:19:A:LEU:HD11 | 20       | 0.29          |
| (1,477) | 1:13:A:TYR:HD1  | 1:19:A:LEU:HD12 | 20       | 0.29          |
| (1,477) | 1:13:A:TYR:HD1  | 1:19:A:LEU:HD13 | 20       | 0.29          |
| (1,477) | 1:13:A:TYR:HD2  | 1:19:A:LEU:HD11 | 20       | 0.29          |
| (1,477) | 1:13:A:TYR:HD2  | 1:19:A:LEU:HD12 | 20       | 0.29          |
| (1,477) | 1:13:A:TYR:HD2  | 1:19:A:LEU:HD13 | 20       | 0.29          |
| (1,281) | 1:12:A:PRO:HD3  | 1:13:A:TYR:HE1  | 20       | 0.29          |
| (1,281) | 1:12:A:PRO:HD3  | 1:13:A:TYR:HE2  | 20       | 0.29          |
| (1,618) | 1:3:A:GLU:HB2   | 1:3:A:GLU:HG2   | 14       | 0.28          |
| (1,618) | 1:3:A:GLU:HB2   | 1:3:A:GLU:HG2   | 18       | 0.28          |
| (1,594) | 1:56:A:ASP:HA   | 1:56:A:ASP:HB2  | 4        | 0.28          |
| (1,594) | 1:56:A:ASP:HA   | 1:56:A:ASP:HB2  | 6        | 0.28          |
| (1,384) | 1:12:A:PRO:HD2  | 1:38:A:GLN:HG2  | 18       | 0.28          |
| (1,384) | 1:12:A:PRO:HD2  | 1:38:A:GLN:HG3  | 18       | 0.28          |
| (1,579) | 1:6:A:TYR:HD1   | 1:17:A:SER:HB2  | 15       | 0.27          |
| (1,579) | 1:6:A:TYR:HD2   | 1:17:A:SER:HB2  | 15       | 0.27          |
| (1,579) | 1:6:A:TYR:HD1   | 1:17:A:SER:HB2  | 19       | 0.27          |
| (1,579) | 1:6:A:TYR:HD2   | 1:17:A:SER:HB2  | 19       | 0.27          |
| (1,594) | 1:56:A:ASP:HA   | 1:56:A:ASP:HB2  | 9        | 0.26          |
| (1,594) | 1:56:A:ASP:HA   | 1:56:A:ASP:HB2  | 10       | 0.26          |
| (1,594) | 1:56:A:ASP:HA   | 1:56:A:ASP:HB2  | 12       | 0.26          |
| (1,439) | 1:12:A:PRO:HG3  | 1:13:A:TYR:HE1  | 14       | 0.26          |
| (1,439) | 1:12:A:PRO:HG3  | 1:13:A:TYR:HE2  | 14       | 0.26          |
| (1,248) | 1:5:A:PHE:HB3   | 1:6:A:TYR:H     | 20       | 0.26          |
| (1,74)  | 1:16:A:ASP:HB2  | 1:18:A:GLN:H    | 3        | 0.26          |
| (1,639) | 1:16:A:ASP:HB2  | 1:19:A:LEU:HB2  | 1        | 0.25          |
| (1,601) | 1:23:A:THR:HG21 | 1:30:A:ASN:HB2  | 7        | 0.25          |
| (1,601) | 1:23:A:THR:HG22 | 1:30:A:ASN:HB2  | 7        | 0.25          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,601) | 1:23:A:THR:HG23 | 1:30:A:ASN:HB2  | 7        | 0.25          |
| (1,536) | 1:21:A:TRP:HZ3  | 1:25:A:SER:HB2  | 1        | 0.25          |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD11 | 7        | 0.25          |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD12 | 7        | 0.25          |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD13 | 7        | 0.25          |
| (1,414) | 1:3:A:GLU:HB3   | 1:4:A:ASP:H     | 12       | 0.25          |
| (1,373) | 1:12:A:PRO:HD2  | 1:38:A:GLN:HB2  | 4        | 0.25          |
| (1,373) | 1:12:A:PRO:HD2  | 1:38:A:GLN:HB3  | 4        | 0.25          |
| (1,248) | 1:5:A:PHE:HB3   | 1:6:A:TYR:H     | 19       | 0.25          |
| (1,688) | 1:11:A:CYS:SG   | 1:39:A:CYS:CB   | 18       | 0.24          |
| (1,594) | 1:56:A:ASP:HA   | 1:56:A:ASP:HB2  | 17       | 0.24          |
| (1,575) | 1:6:A:TYR:HE1   | 1:17:A:SER:HB2  | 10       | 0.24          |
| (1,575) | 1:6:A:TYR:HE2   | 1:17:A:SER:HB2  | 10       | 0.24          |
| (1,294) | 1:17:A:SER:HA   | 1:17:A:SER:HB3  | 7        | 0.24          |
| (1,294) | 1:17:A:SER:HA   | 1:17:A:SER:HB3  | 17       | 0.24          |
| (1,294) | 1:17:A:SER:HA   | 1:17:A:SER:HB3  | 20       | 0.24          |
| (1,281) | 1:12:A:PRO:HD3  | 1:13:A:TYR:HE1  | 1        | 0.24          |
| (1,281) | 1:12:A:PRO:HD3  | 1:13:A:TYR:HE2  | 1        | 0.24          |
| (1,618) | 1:3:A:GLU:HB2   | 1:3:A:GLU:HG2   | 1        | 0.23          |
| (1,618) | 1:3:A:GLU:HB2   | 1:3:A:GLU:HG2   | 5        | 0.23          |
| (1,618) | 1:3:A:GLU:HB2   | 1:3:A:GLU:HG2   | 15       | 0.23          |
| (1,601) | 1:23:A:THR:HG21 | 1:30:A:ASN:HB2  | 13       | 0.23          |
| (1,601) | 1:23:A:THR:HG22 | 1:30:A:ASN:HB2  | 13       | 0.23          |
| (1,601) | 1:23:A:THR:HG23 | 1:30:A:ASN:HB2  | 13       | 0.23          |
| (1,581) | 1:3:A:GLU:HB2   | 1:17:A:SER:HB2  | 15       | 0.23          |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD11 | 17       | 0.23          |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD12 | 17       | 0.23          |
| (1,479) | 1:14:A:LYS:HE2  | 1:19:A:LEU:HD13 | 17       | 0.23          |
| (1,478) | 1:13:A:TYR:HB3  | 1:19:A:LEU:HD11 | 7        | 0.23          |
| (1,478) | 1:13:A:TYR:HB3  | 1:19:A:LEU:HD12 | 7        | 0.23          |
| (1,478) | 1:13:A:TYR:HB3  | 1:19:A:LEU:HD13 | 7        | 0.23          |
| (1,414) | 1:3:A:GLU:HB3   | 1:4:A:ASP:H     | 2        | 0.23          |
| (1,248) | 1:5:A:PHE:HB3   | 1:6:A:TYR:H     | 8        | 0.23          |
| (1,248) | 1:5:A:PHE:HB3   | 1:6:A:TYR:H     | 15       | 0.23          |
| (1,688) | 1:11:A:CYS:SG   | 1:39:A:CYS:CB   | 19       | 0.22          |
| (1,688) | 1:11:A:CYS:SG   | 1:39:A:CYS:CB   | 20       | 0.22          |
| (1,639) | 1:16:A:ASP:HB2  | 1:19:A:LEU:HB2  | 14       | 0.22          |
| (1,618) | 1:3:A:GLU:HB2   | 1:3:A:GLU:HG2   | 7        | 0.22          |
| (1,594) | 1:56:A:ASP:HA   | 1:56:A:ASP:HB2  | 14       | 0.22          |
| (1,579) | 1:6:A:TYR:HD1   | 1:17:A:SER:HB2  | 3        | 0.22          |
| (1,579) | 1:6:A:TYR:HD2   | 1:17:A:SER:HB2  | 3        | 0.22          |
| (1,554) | 1:19:A:LEU:HD11 | 1:20:A:ALA:HA   | 6        | 0.22          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,554) | 1:19:A:LEU:HD12 | 1:20:A:ALA:HA   | 6        | 0.22          |
| (1,554) | 1:19:A:LEU:HD13 | 1:20:A:ALA:HA   | 6        | 0.22          |
| (1,541) | 1:6:A:TYR:HA    | 1:17:A:SER:HB2  | 1        | 0.22          |
| (1,481) | 1:16:A:ASP:HB3  | 1:19:A:LEU:HD11 | 13       | 0.22          |
| (1,481) | 1:16:A:ASP:HB3  | 1:19:A:LEU:HD12 | 13       | 0.22          |
| (1,481) | 1:16:A:ASP:HB3  | 1:19:A:LEU:HD13 | 13       | 0.22          |
| (1,477) | 1:13:A:TYR:HD1  | 1:19:A:LEU:HD11 | 13       | 0.22          |
| (1,477) | 1:13:A:TYR:HD1  | 1:19:A:LEU:HD12 | 13       | 0.22          |
| (1,477) | 1:13:A:TYR:HD1  | 1:19:A:LEU:HD13 | 13       | 0.22          |
| (1,477) | 1:13:A:TYR:HD2  | 1:19:A:LEU:HD11 | 13       | 0.22          |
| (1,477) | 1:13:A:TYR:HD2  | 1:19:A:LEU:HD12 | 13       | 0.22          |
| (1,477) | 1:13:A:TYR:HD2  | 1:19:A:LEU:HD13 | 13       | 0.22          |
| (1,414) | 1:3:A:GLU:HB3   | 1:4:A:ASP:H     | 11       | 0.22          |
| (1,414) | 1:3:A:GLU:HB3   | 1:4:A:ASP:H     | 14       | 0.22          |
| (1,414) | 1:3:A:GLU:HB3   | 1:4:A:ASP:H     | 18       | 0.22          |
| (1,414) | 1:3:A:GLU:HB3   | 1:4:A:ASP:H     | 19       | 0.22          |
| (1,366) | 1:24:A:CYS:HB3  | 1:35:A:CYS:HB2  | 18       | 0.22          |
| (1,366) | 1:24:A:CYS:HB3  | 1:35:A:CYS:HB2  | 19       | 0.22          |
| (1,294) | 1:17:A:SER:HA   | 1:17:A:SER:HB3  | 13       | 0.22          |
| (1,248) | 1:5:A:PHE:HB3   | 1:6:A:TYR:H     | 11       | 0.22          |
| (1,248) | 1:5:A:PHE:HB3   | 1:6:A:TYR:H     | 14       | 0.22          |
| (1,605) | 1:27:A:GLY:HA3  | 1:53:A:ASP:HB2  | 14       | 0.21          |
| (1,605) | 1:27:A:GLY:HA3  | 1:53:A:ASP:HB3  | 14       | 0.21          |
| (1,575) | 1:6:A:TYR:HE1   | 1:17:A:SER:HB2  | 11       | 0.21          |
| (1,575) | 1:6:A:TYR:HE2   | 1:17:A:SER:HB2  | 11       | 0.21          |
| (1,575) | 1:6:A:TYR:HE1   | 1:17:A:SER:HB2  | 12       | 0.21          |
| (1,575) | 1:6:A:TYR:HE2   | 1:17:A:SER:HB2  | 12       | 0.21          |
| (1,566) | 1:34:A:VAL:HA   | 1:38:A:GLN:HB2  | 17       | 0.21          |
| (1,566) | 1:34:A:VAL:HA   | 1:38:A:GLN:HB3  | 17       | 0.21          |
| (1,281) | 1:12:A:PRO:HD3  | 1:13:A:TYR:HE1  | 11       | 0.21          |
| (1,281) | 1:12:A:PRO:HD3  | 1:13:A:TYR:HE2  | 11       | 0.21          |
| (1,248) | 1:5:A:PHE:HB3   | 1:6:A:TYR:H     | 4        | 0.21          |
| (1,248) | 1:5:A:PHE:HB3   | 1:6:A:TYR:H     | 5        | 0.21          |
| (1,248) | 1:5:A:PHE:HB3   | 1:6:A:TYR:H     | 18       | 0.21          |
| (1,74)  | 1:16:A:ASP:HB2  | 1:18:A:GLN:H    | 11       | 0.21          |
| (1,74)  | 1:16:A:ASP:HB2  | 1:18:A:GLN:H    | 18       | 0.21          |
| (1,607) | 1:16:A:ASP:HB2  | 1:19:A:LEU:HB3  | 6        | 0.2           |
| (1,566) | 1:34:A:VAL:HA   | 1:38:A:GLN:HB2  | 4        | 0.2           |
| (1,566) | 1:34:A:VAL:HA   | 1:38:A:GLN:HB3  | 4        | 0.2           |
| (1,554) | 1:19:A:LEU:HD11 | 1:20:A:ALA:HA   | 4        | 0.2           |
| (1,554) | 1:19:A:LEU:HD12 | 1:20:A:ALA:HA   | 4        | 0.2           |
| (1,554) | 1:19:A:LEU:HD13 | 1:20:A:ALA:HA   | 4        | 0.2           |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,536) | 1:21:A:TRP:HZ3 | 1:25:A:SER:HB2 | 4        | 0.2           |
| (1,414) | 1:3:A:GLU:HB3  | 1:4:A:ASP:H    | 16       | 0.2           |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB2 | 16       | 0.2           |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB3 | 16       | 0.2           |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB2 | 20       | 0.2           |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB3 | 20       | 0.2           |
| (1,281) | 1:12:A:PRO:HD3 | 1:13:A:TYR:HE1 | 15       | 0.2           |
| (1,281) | 1:12:A:PRO:HD3 | 1:13:A:TYR:HE2 | 15       | 0.2           |
| (1,248) | 1:5:A:PHE:HB3  | 1:6:A:TYR:H    | 1        | 0.2           |
| (1,248) | 1:5:A:PHE:HB3  | 1:6:A:TYR:H    | 2        | 0.2           |
| (1,248) | 1:5:A:PHE:HB3  | 1:6:A:TYR:H    | 3        | 0.2           |
| (1,248) | 1:5:A:PHE:HB3  | 1:6:A:TYR:H    | 10       | 0.2           |
| (1,248) | 1:5:A:PHE:HB3  | 1:6:A:TYR:H    | 12       | 0.2           |
| (1,248) | 1:5:A:PHE:HB3  | 1:6:A:TYR:H    | 13       | 0.2           |
| (1,98)  | 1:51:A:MET:HG3 | 1:53:A:ASP:H   | 17       | 0.2           |
| (1,641) | 1:19:A:LEU:HB3 | 1:20:A:ALA:HA  | 18       | 0.19          |
| (1,414) | 1:3:A:GLU:HB3  | 1:4:A:ASP:H    | 4        | 0.19          |
| (1,414) | 1:3:A:GLU:HB3  | 1:4:A:ASP:H    | 10       | 0.19          |
| (1,373) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HB2 | 9        | 0.19          |
| (1,373) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HB3 | 9        | 0.19          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB2 | 5        | 0.19          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB3 | 5        | 0.19          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB2 | 6        | 0.19          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB3 | 6        | 0.19          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB2 | 8        | 0.19          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB3 | 8        | 0.19          |
| (1,248) | 1:5:A:PHE:HB3  | 1:6:A:TYR:H    | 7        | 0.19          |
| (1,248) | 1:5:A:PHE:HB3  | 1:6:A:TYR:H    | 17       | 0.19          |
| (1,74)  | 1:16:A:ASP:HB2 | 1:18:A:GLN:H   | 2        | 0.19          |
| (1,74)  | 1:16:A:ASP:HB2 | 1:18:A:GLN:H   | 5        | 0.19          |
| (1,692) | 1:35:A:CYS:SG  | 1:48:A:CYS:CB  | 6        | 0.18          |
| (1,575) | 1:6:A:TYR:HE1  | 1:17:A:SER:HB2 | 8        | 0.18          |
| (1,575) | 1:6:A:TYR:HE2  | 1:17:A:SER:HB2 | 8        | 0.18          |
| (1,575) | 1:6:A:TYR:HE1  | 1:17:A:SER:HB2 | 19       | 0.18          |
| (1,575) | 1:6:A:TYR:HE2  | 1:17:A:SER:HB2 | 19       | 0.18          |
| (1,566) | 1:34:A:VAL:HA  | 1:38:A:GLN:HB2 | 9        | 0.18          |
| (1,566) | 1:34:A:VAL:HA  | 1:38:A:GLN:HB3 | 9        | 0.18          |
| (1,566) | 1:34:A:VAL:HA  | 1:38:A:GLN:HB2 | 12       | 0.18          |
| (1,566) | 1:34:A:VAL:HA  | 1:38:A:GLN:HB3 | 12       | 0.18          |
| (1,566) | 1:34:A:VAL:HA  | 1:38:A:GLN:HB2 | 13       | 0.18          |
| (1,566) | 1:34:A:VAL:HA  | 1:38:A:GLN:HB3 | 13       | 0.18          |
| (1,565) | 1:36:A:CYS:HB3 | 1:45:A:SER:HA  | 15       | 0.18          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,547) | 1:53:A:ASP:HA  | 1:54:A:SER:HA   | 3        | 0.18          |
| (1,547) | 1:53:A:ASP:HA  | 1:54:A:SER:HA   | 10       | 0.18          |
| (1,541) | 1:6:A:TYR:HA   | 1:17:A:SER:HB2  | 4        | 0.18          |
| (1,536) | 1:21:A:TRP:HZ3 | 1:25:A:SER:HB2  | 12       | 0.18          |
| (1,479) | 1:14:A:LYS:HE2 | 1:19:A:LEU:HD11 | 9        | 0.18          |
| (1,479) | 1:14:A:LYS:HE2 | 1:19:A:LEU:HD12 | 9        | 0.18          |
| (1,479) | 1:14:A:LYS:HE2 | 1:19:A:LEU:HD13 | 9        | 0.18          |
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD11 | 17       | 0.18          |
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD12 | 17       | 0.18          |
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD13 | 17       | 0.18          |
| (1,414) | 1:3:A:GLU:HB3  | 1:4:A:ASP:H     | 9        | 0.18          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB2  | 9        | 0.18          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB3  | 9        | 0.18          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB2  | 10       | 0.18          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB3  | 10       | 0.18          |
| (1,283) | 1:25:A:SER:HB2 | 1:51:A:MET:H    | 19       | 0.18          |
| (1,248) | 1:5:A:PHE:HB3  | 1:6:A:TYR:H     | 9        | 0.18          |
| (1,175) | 1:52:A:ALA:HB1 | 1:53:A:ASP:HA   | 17       | 0.18          |
| (1,175) | 1:52:A:ALA:HB2 | 1:53:A:ASP:HA   | 17       | 0.18          |
| (1,175) | 1:52:A:ALA:HB3 | 1:53:A:ASP:HA   | 17       | 0.18          |
| (1,66)  | 1:27:A:GLY:H   | 1:53:A:ASP:HB2  | 19       | 0.18          |
| (1,66)  | 1:27:A:GLY:H   | 1:53:A:ASP:HB3  | 19       | 0.18          |
| (1,692) | 1:35:A:CYS:SG  | 1:48:A:CYS:CB   | 19       | 0.17          |
| (1,581) | 1:3:A:GLU:HB2  | 1:17:A:SER:HB2  | 5        | 0.17          |
| (1,566) | 1:34:A:VAL:HA  | 1:38:A:GLN:HB2  | 16       | 0.17          |
| (1,566) | 1:34:A:VAL:HA  | 1:38:A:GLN:HB3  | 16       | 0.17          |
| (1,481) | 1:16:A:ASP:HB3 | 1:19:A:LEU:HD11 | 20       | 0.17          |
| (1,481) | 1:16:A:ASP:HB3 | 1:19:A:LEU:HD12 | 20       | 0.17          |
| (1,481) | 1:16:A:ASP:HB3 | 1:19:A:LEU:HD13 | 20       | 0.17          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB2  | 19       | 0.17          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB3  | 19       | 0.17          |
| (1,360) | 1:22:A:ASP:HB2 | 1:23:A:THR:H    | 6        | 0.17          |
| (1,248) | 1:5:A:PHE:HB3  | 1:6:A:TYR:H     | 16       | 0.17          |
| (1,175) | 1:52:A:ALA:HB1 | 1:53:A:ASP:HA   | 12       | 0.17          |
| (1,175) | 1:52:A:ALA:HB2 | 1:53:A:ASP:HA   | 12       | 0.17          |
| (1,175) | 1:52:A:ALA:HB3 | 1:53:A:ASP:HA   | 12       | 0.17          |
| (1,74)  | 1:16:A:ASP:HB2 | 1:18:A:GLN:H    | 20       | 0.17          |
| (1,50)  | 1:25:A:SER:HA  | 1:52:A:ALA:H    | 10       | 0.17          |
| (1,579) | 1:6:A:TYR:HD1  | 1:17:A:SER:HB2  | 5        | 0.16          |
| (1,579) | 1:6:A:TYR:HD2  | 1:17:A:SER:HB2  | 5        | 0.16          |
| (1,414) | 1:3:A:GLU:HB3  | 1:4:A:ASP:H     | 3        | 0.16          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB2  | 3        | 0.16          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB3  | 3        | 0.16          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB2  | 7        | 0.16          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB3  | 7        | 0.16          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB2  | 15       | 0.16          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB3  | 15       | 0.16          |
| (1,366) | 1:24:A:CYS:HB3 | 1:35:A:CYS:HB2  | 1        | 0.16          |
| (1,175) | 1:52:A:ALA:HB1 | 1:53:A:ASP:HA   | 6        | 0.16          |
| (1,175) | 1:52:A:ALA:HB2 | 1:53:A:ASP:HA   | 6        | 0.16          |
| (1,175) | 1:52:A:ALA:HB3 | 1:53:A:ASP:HA   | 6        | 0.16          |
| (1,175) | 1:52:A:ALA:HB1 | 1:53:A:ASP:HA   | 11       | 0.16          |
| (1,175) | 1:52:A:ALA:HB2 | 1:53:A:ASP:HA   | 11       | 0.16          |
| (1,175) | 1:52:A:ALA:HB3 | 1:53:A:ASP:HA   | 11       | 0.16          |
| (1,175) | 1:52:A:ALA:HB1 | 1:53:A:ASP:HA   | 18       | 0.16          |
| (1,175) | 1:52:A:ALA:HB2 | 1:53:A:ASP:HA   | 18       | 0.16          |
| (1,175) | 1:52:A:ALA:HB3 | 1:53:A:ASP:HA   | 18       | 0.16          |
| (1,692) | 1:35:A:CYS:SG  | 1:48:A:CYS:CB   | 18       | 0.15          |
| (1,641) | 1:19:A:LEU:HB3 | 1:20:A:ALA:HA   | 8        | 0.15          |
| (1,639) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HB2  | 2        | 0.15          |
| (1,636) | 1:32:A:GLY:HA3 | 1:52:A:ALA:HB1  | 17       | 0.15          |
| (1,636) | 1:32:A:GLY:HA3 | 1:52:A:ALA:HB2  | 17       | 0.15          |
| (1,636) | 1:32:A:GLY:HA3 | 1:52:A:ALA:HB3  | 17       | 0.15          |
| (1,547) | 1:53:A:ASP:HA  | 1:54:A:SER:HA   | 17       | 0.15          |
| (1,541) | 1:6:A:TYR:HA   | 1:17:A:SER:HB2  | 15       | 0.15          |
| (1,477) | 1:13:A:TYR:HD1 | 1:19:A:LEU:HD11 | 2        | 0.15          |
| (1,477) | 1:13:A:TYR:HD1 | 1:19:A:LEU:HD12 | 2        | 0.15          |
| (1,477) | 1:13:A:TYR:HD1 | 1:19:A:LEU:HD13 | 2        | 0.15          |
| (1,477) | 1:13:A:TYR:HD2 | 1:19:A:LEU:HD11 | 2        | 0.15          |
| (1,477) | 1:13:A:TYR:HD2 | 1:19:A:LEU:HD12 | 2        | 0.15          |
| (1,477) | 1:13:A:TYR:HD2 | 1:19:A:LEU:HD13 | 2        | 0.15          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB2  | 12       | 0.15          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB3  | 12       | 0.15          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB2  | 14       | 0.15          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB3  | 14       | 0.15          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB2  | 18       | 0.15          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB3  | 18       | 0.15          |
| (1,251) | 1:26:A:GLY:HA2 | 1:28:A:THR:H    | 8        | 0.15          |
| (1,248) | 1:5:A:PHE:HB3  | 1:6:A:TYR:H     | 6        | 0.15          |
| (1,175) | 1:52:A:ALA:HB1 | 1:53:A:ASP:HA   | 14       | 0.15          |
| (1,175) | 1:52:A:ALA:HB2 | 1:53:A:ASP:HA   | 14       | 0.15          |
| (1,175) | 1:52:A:ALA:HB3 | 1:53:A:ASP:HA   | 14       | 0.15          |
| (1,692) | 1:35:A:CYS:SG  | 1:48:A:CYS:CB   | 15       | 0.14          |
| (1,641) | 1:19:A:LEU:HB3 | 1:20:A:ALA:HA   | 10       | 0.14          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,639) | 1:16:A:ASP:HB2 | 1:19:A:LEU:HB2  | 19       | 0.14          |
| (1,575) | 1:6:A:TYR:HE1  | 1:17:A:SER:HB2  | 15       | 0.14          |
| (1,575) | 1:6:A:TYR:HE2  | 1:17:A:SER:HB2  | 15       | 0.14          |
| (1,541) | 1:6:A:TYR:HA   | 1:17:A:SER:HB2  | 19       | 0.14          |
| (1,414) | 1:3:A:GLU:HB3  | 1:4:A:ASP:H     | 8        | 0.14          |
| (1,389) | 1:21:A:TRP:HH2 | 1:25:A:SER:HB3  | 17       | 0.14          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB2  | 11       | 0.14          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB3  | 11       | 0.14          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB2  | 17       | 0.14          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB3  | 17       | 0.14          |
| (1,366) | 1:24:A:CYS:HB3 | 1:35:A:CYS:HB2  | 3        | 0.14          |
| (1,251) | 1:26:A:GLY:HA2 | 1:28:A:THR:H    | 3        | 0.14          |
| (1,175) | 1:52:A:ALA:HB1 | 1:53:A:ASP:HA   | 16       | 0.14          |
| (1,175) | 1:52:A:ALA:HB2 | 1:53:A:ASP:HA   | 16       | 0.14          |
| (1,175) | 1:52:A:ALA:HB3 | 1:53:A:ASP:HA   | 16       | 0.14          |
| (1,80)  | 1:35:A:CYS:H   | 1:35:A:CYS:HB2  | 5        | 0.14          |
| (1,80)  | 1:35:A:CYS:H   | 1:35:A:CYS:HB2  | 6        | 0.14          |
| (1,80)  | 1:35:A:CYS:H   | 1:35:A:CYS:HB2  | 8        | 0.14          |
| (1,80)  | 1:35:A:CYS:H   | 1:35:A:CYS:HB2  | 19       | 0.14          |
| (1,46)  | 1:37:A:GLY:H   | 1:45:A:SER:HB2  | 2        | 0.14          |
| (1,46)  | 1:37:A:GLY:H   | 1:45:A:SER:HB3  | 2        | 0.14          |
| (1,692) | 1:35:A:CYS:SG  | 1:48:A:CYS:CB   | 3        | 0.13          |
| (1,692) | 1:35:A:CYS:SG  | 1:48:A:CYS:CB   | 7        | 0.13          |
| (1,692) | 1:35:A:CYS:SG  | 1:48:A:CYS:CB   | 8        | 0.13          |
| (1,692) | 1:35:A:CYS:SG  | 1:48:A:CYS:CB   | 16       | 0.13          |
| (1,669) | 1:21:A:TRP:HE3 | 1:44:A:VAL:HG11 | 7        | 0.13          |
| (1,669) | 1:21:A:TRP:HE3 | 1:44:A:VAL:HG12 | 7        | 0.13          |
| (1,669) | 1:21:A:TRP:HE3 | 1:44:A:VAL:HG13 | 7        | 0.13          |
| (1,641) | 1:19:A:LEU:HB3 | 1:20:A:ALA:HA   | 3        | 0.13          |
| (1,641) | 1:19:A:LEU:HB3 | 1:20:A:ALA:HA   | 5        | 0.13          |
| (1,641) | 1:19:A:LEU:HB3 | 1:20:A:ALA:HA   | 15       | 0.13          |
| (1,575) | 1:6:A:TYR:HE1  | 1:17:A:SER:HB2  | 3        | 0.13          |
| (1,575) | 1:6:A:TYR:HE2  | 1:17:A:SER:HB2  | 3        | 0.13          |
| (1,565) | 1:36:A:CYS:HB3 | 1:45:A:SER:HA   | 11       | 0.13          |
| (1,547) | 1:53:A:ASP:HA  | 1:54:A:SER:HA   | 2        | 0.13          |
| (1,547) | 1:53:A:ASP:HA  | 1:54:A:SER:HA   | 19       | 0.13          |
| (1,481) | 1:16:A:ASP:HB3 | 1:19:A:LEU:HD11 | 9        | 0.13          |
| (1,481) | 1:16:A:ASP:HB3 | 1:19:A:LEU:HD12 | 9        | 0.13          |
| (1,481) | 1:16:A:ASP:HB3 | 1:19:A:LEU:HD13 | 9        | 0.13          |
| (1,481) | 1:16:A:ASP:HB3 | 1:19:A:LEU:HD11 | 19       | 0.13          |
| (1,481) | 1:16:A:ASP:HB3 | 1:19:A:LEU:HD12 | 19       | 0.13          |
| (1,481) | 1:16:A:ASP:HB3 | 1:19:A:LEU:HD13 | 19       | 0.13          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD11 | 16       | 0.13          |
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD12 | 16       | 0.13          |
| (1,478) | 1:13:A:TYR:HB3 | 1:19:A:LEU:HD13 | 16       | 0.13          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB2  | 1        | 0.13          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB3  | 1        | 0.13          |
| (1,353) | 1:6:A:TYR:HE1  | 1:39:A:CYS:HB3  | 20       | 0.13          |
| (1,353) | 1:6:A:TYR:HE2  | 1:39:A:CYS:HB3  | 20       | 0.13          |
| (1,318) | 1:14:A:LYS:HE3 | 1:15:A:ASN:HB2  | 18       | 0.13          |
| (1,279) | 1:12:A:PRO:HD3 | 1:13:A:TYR:HD1  | 7        | 0.13          |
| (1,279) | 1:12:A:PRO:HD3 | 1:13:A:TYR:HD2  | 7        | 0.13          |
| (1,175) | 1:52:A:ALA:HB1 | 1:53:A:ASP:HA   | 4        | 0.13          |
| (1,175) | 1:52:A:ALA:HB2 | 1:53:A:ASP:HA   | 4        | 0.13          |
| (1,175) | 1:52:A:ALA:HB3 | 1:53:A:ASP:HA   | 4        | 0.13          |
| (1,80)  | 1:35:A:CYS:H   | 1:35:A:CYS:HB2  | 10       | 0.13          |
| (1,80)  | 1:35:A:CYS:H   | 1:35:A:CYS:HB2  | 15       | 0.13          |
| (1,50)  | 1:25:A:SER:HA  | 1:52:A:ALA:H    | 9        | 0.13          |
| (1,46)  | 1:37:A:GLY:H   | 1:45:A:SER:HB2  | 11       | 0.13          |
| (1,46)  | 1:37:A:GLY:H   | 1:45:A:SER:HB3  | 11       | 0.13          |
| (1,618) | 1:3:A:GLU:HB2  | 1:3:A:GLU:HG2   | 16       | 0.12          |
| (1,612) | 1:30:A:ASN:HA  | 1:30:A:ASN:HB3  | 5        | 0.12          |
| (1,609) | 1:11:A:CYS:HA  | 1:38:A:GLN:HB2  | 6        | 0.12          |
| (1,609) | 1:11:A:CYS:HA  | 1:38:A:GLN:HB3  | 6        | 0.12          |
| (1,609) | 1:11:A:CYS:HA  | 1:38:A:GLN:HB2  | 19       | 0.12          |
| (1,609) | 1:11:A:CYS:HA  | 1:38:A:GLN:HB3  | 19       | 0.12          |
| (1,565) | 1:36:A:CYS:HB3 | 1:45:A:SER:HA   | 2        | 0.12          |
| (1,547) | 1:53:A:ASP:HA  | 1:54:A:SER:HA   | 6        | 0.12          |
| (1,547) | 1:53:A:ASP:HA  | 1:54:A:SER:HA   | 8        | 0.12          |
| (1,547) | 1:53:A:ASP:HA  | 1:54:A:SER:HA   | 9        | 0.12          |
| (1,547) | 1:53:A:ASP:HA  | 1:54:A:SER:HA   | 11       | 0.12          |
| (1,547) | 1:53:A:ASP:HA  | 1:54:A:SER:HA   | 14       | 0.12          |
| (1,547) | 1:53:A:ASP:HA  | 1:54:A:SER:HA   | 15       | 0.12          |
| (1,547) | 1:53:A:ASP:HA  | 1:54:A:SER:HA   | 18       | 0.12          |
| (1,541) | 1:6:A:TYR:HA   | 1:17:A:SER:HB2  | 12       | 0.12          |
| (1,385) | 1:3:A:GLU:H    | 1:3:A:GLU:HG2   | 13       | 0.12          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB2  | 13       | 0.12          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB3  | 13       | 0.12          |
| (1,366) | 1:24:A:CYS:HB3 | 1:35:A:CYS:HB2  | 14       | 0.12          |
| (1,350) | 1:52:A:ALA:H   | 1:53:A:ASP:HB2  | 17       | 0.12          |
| (1,350) | 1:52:A:ALA:H   | 1:53:A:ASP:HB3  | 17       | 0.12          |
| (1,263) | 1:44:A:VAL:HA  | 1:48:A:CYS:H    | 8        | 0.12          |
| (1,198) | 1:41:A:SER:H   | 1:41:A:SER:HB2  | 2        | 0.12          |
| (1,198) | 1:41:A:SER:H   | 1:41:A:SER:HB2  | 7        | 0.12          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,198) | 1:41:A:SER:H   | 1:41:A:SER:HB2  | 18       | 0.12          |
| (1,181) | 1:9:A:GLU:HB3  | 1:10:A:THR:HB   | 15       | 0.12          |
| (1,175) | 1:52:A:ALA:HB1 | 1:53:A:ASP:HA   | 1        | 0.12          |
| (1,175) | 1:52:A:ALA:HB2 | 1:53:A:ASP:HA   | 1        | 0.12          |
| (1,175) | 1:52:A:ALA:HB3 | 1:53:A:ASP:HA   | 1        | 0.12          |
| (1,175) | 1:52:A:ALA:HB1 | 1:53:A:ASP:HA   | 3        | 0.12          |
| (1,175) | 1:52:A:ALA:HB2 | 1:53:A:ASP:HA   | 3        | 0.12          |
| (1,175) | 1:52:A:ALA:HB3 | 1:53:A:ASP:HA   | 3        | 0.12          |
| (1,175) | 1:52:A:ALA:HB1 | 1:53:A:ASP:HA   | 7        | 0.12          |
| (1,175) | 1:52:A:ALA:HB2 | 1:53:A:ASP:HA   | 7        | 0.12          |
| (1,175) | 1:52:A:ALA:HB3 | 1:53:A:ASP:HA   | 7        | 0.12          |
| (1,175) | 1:52:A:ALA:HB1 | 1:53:A:ASP:HA   | 15       | 0.12          |
| (1,175) | 1:52:A:ALA:HB2 | 1:53:A:ASP:HA   | 15       | 0.12          |
| (1,175) | 1:52:A:ALA:HB3 | 1:53:A:ASP:HA   | 15       | 0.12          |
| (1,175) | 1:52:A:ALA:HB1 | 1:53:A:ASP:HA   | 20       | 0.12          |
| (1,175) | 1:52:A:ALA:HB2 | 1:53:A:ASP:HA   | 20       | 0.12          |
| (1,175) | 1:52:A:ALA:HB3 | 1:53:A:ASP:HA   | 20       | 0.12          |
| (1,142) | 1:25:A:SER:H   | 1:26:A:GLY:H    | 12       | 0.12          |
| (1,80)  | 1:35:A:CYS:H   | 1:35:A:CYS:HB2  | 11       | 0.12          |
| (1,80)  | 1:35:A:CYS:H   | 1:35:A:CYS:HB2  | 16       | 0.12          |
| (1,80)  | 1:35:A:CYS:H   | 1:35:A:CYS:HB2  | 18       | 0.12          |
| (1,74)  | 1:16:A:ASP:HB2 | 1:18:A:GLN:H    | 9        | 0.12          |
| (1,50)  | 1:25:A:SER:HA  | 1:52:A:ALA:H    | 5        | 0.12          |
| (1,50)  | 1:25:A:SER:HA  | 1:52:A:ALA:H    | 17       | 0.12          |
| (1,46)  | 1:37:A:GLY:H   | 1:45:A:SER:HB2  | 1        | 0.12          |
| (1,46)  | 1:37:A:GLY:H   | 1:45:A:SER:HB3  | 1        | 0.12          |
| (1,43)  | 1:16:A:ASP:H   | 1:17:A:SER:HA   | 14       | 0.12          |
| (1,693) | 1:35:A:CYS:CB  | 1:48:A:CYS:SG   | 15       | 0.11          |
| (1,692) | 1:35:A:CYS:SG  | 1:48:A:CYS:CB   | 9        | 0.11          |
| (1,692) | 1:35:A:CYS:SG  | 1:48:A:CYS:CB   | 12       | 0.11          |
| (1,692) | 1:35:A:CYS:SG  | 1:48:A:CYS:CB   | 20       | 0.11          |
| (1,669) | 1:21:A:TRP:HE3 | 1:44:A:VAL:HG11 | 17       | 0.11          |
| (1,669) | 1:21:A:TRP:HE3 | 1:44:A:VAL:HG12 | 17       | 0.11          |
| (1,669) | 1:21:A:TRP:HE3 | 1:44:A:VAL:HG13 | 17       | 0.11          |
| (1,612) | 1:30:A:ASN:HA  | 1:30:A:ASN:HB3  | 7        | 0.11          |
| (1,609) | 1:11:A:CYS:HA  | 1:38:A:GLN:HB2  | 8        | 0.11          |
| (1,609) | 1:11:A:CYS:HA  | 1:38:A:GLN:HB3  | 8        | 0.11          |
| (1,605) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HB2  | 4        | 0.11          |
| (1,605) | 1:27:A:GLY:HA3 | 1:53:A:ASP:HB3  | 4        | 0.11          |
| (1,559) | 1:54:A:SER:HA  | 1:54:A:SER:HB2  | 6        | 0.11          |
| (1,559) | 1:54:A:SER:HA  | 1:54:A:SER:HB2  | 11       | 0.11          |
| (1,559) | 1:54:A:SER:HA  | 1:54:A:SER:HB2  | 12       | 0.11          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,559) | 1:54:A:SER:HA  | 1:54:A:SER:HB2 | 18       | 0.11          |
| (1,547) | 1:53:A:ASP:HA  | 1:54:A:SER:HA  | 1        | 0.11          |
| (1,547) | 1:53:A:ASP:HA  | 1:54:A:SER:HA  | 4        | 0.11          |
| (1,547) | 1:53:A:ASP:HA  | 1:54:A:SER:HA  | 5        | 0.11          |
| (1,547) | 1:53:A:ASP:HA  | 1:54:A:SER:HA  | 7        | 0.11          |
| (1,547) | 1:53:A:ASP:HA  | 1:54:A:SER:HA  | 12       | 0.11          |
| (1,547) | 1:53:A:ASP:HA  | 1:54:A:SER:HA  | 20       | 0.11          |
| (1,541) | 1:6:A:TYR:HA   | 1:17:A:SER:HB2 | 2        | 0.11          |
| (1,536) | 1:21:A:TRP:HZ3 | 1:25:A:SER:HB2 | 10       | 0.11          |
| (1,488) | 1:7:A:THR:HG21 | 1:11:A:CYS:H   | 16       | 0.11          |
| (1,488) | 1:7:A:THR:HG22 | 1:11:A:CYS:H   | 16       | 0.11          |
| (1,488) | 1:7:A:THR:HG23 | 1:11:A:CYS:H   | 16       | 0.11          |
| (1,483) | 1:7:A:THR:HG21 | 1:41:A:SER:H   | 14       | 0.11          |
| (1,483) | 1:7:A:THR:HG22 | 1:41:A:SER:H   | 14       | 0.11          |
| (1,483) | 1:7:A:THR:HG23 | 1:41:A:SER:H   | 14       | 0.11          |
| (1,473) | 1:13:A:TYR:HB2 | 1:19:A:LEU:HG  | 18       | 0.11          |
| (1,435) | 1:14:A:LYS:H   | 1:14:A:LYS:HB2 | 9        | 0.11          |
| (1,435) | 1:14:A:LYS:H   | 1:14:A:LYS:HB3 | 9        | 0.11          |
| (1,435) | 1:14:A:LYS:H   | 1:14:A:LYS:HB2 | 16       | 0.11          |
| (1,435) | 1:14:A:LYS:H   | 1:14:A:LYS:HB3 | 16       | 0.11          |
| (1,385) | 1:3:A:GLU:H    | 1:3:A:GLU:HG2  | 17       | 0.11          |
| (1,373) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HB2 | 17       | 0.11          |
| (1,373) | 1:12:A:PRO:HD2 | 1:38:A:GLN:HB3 | 17       | 0.11          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB2 | 2        | 0.11          |
| (1,370) | 1:40:A:PHE:HB3 | 1:45:A:SER:HB3 | 2        | 0.11          |
| (1,360) | 1:22:A:ASP:HB2 | 1:23:A:THR:H   | 20       | 0.11          |
| (1,353) | 1:6:A:TYR:HE1  | 1:39:A:CYS:HB3 | 18       | 0.11          |
| (1,353) | 1:6:A:TYR:HE2  | 1:39:A:CYS:HB3 | 18       | 0.11          |
| (1,279) | 1:12:A:PRO:HD3 | 1:13:A:TYR:HD1 | 14       | 0.11          |
| (1,279) | 1:12:A:PRO:HD3 | 1:13:A:TYR:HD2 | 14       | 0.11          |
| (1,278) | 1:23:A:THR:HA  | 1:23:A:THR:HB  | 19       | 0.11          |
| (1,263) | 1:44:A:VAL:HA  | 1:48:A:CYS:H   | 6        | 0.11          |
| (1,181) | 1:9:A:GLU:HB3  | 1:10:A:THR:HB  | 14       | 0.11          |
| (1,98)  | 1:51:A:MET:HG3 | 1:53:A:ASP:H   | 8        | 0.11          |
| (1,80)  | 1:35:A:CYS:H   | 1:35:A:CYS:HB2 | 2        | 0.11          |
| (1,80)  | 1:35:A:CYS:H   | 1:35:A:CYS:HB2 | 3        | 0.11          |
| (1,74)  | 1:16:A:ASP:HB2 | 1:18:A:GLN:H   | 6        | 0.11          |
| (1,74)  | 1:16:A:ASP:HB2 | 1:18:A:GLN:H   | 12       | 0.11          |
| (1,50)  | 1:25:A:SER:HA  | 1:52:A:ALA:H   | 1        | 0.11          |
| (1,50)  | 1:25:A:SER:HA  | 1:52:A:ALA:H   | 8        | 0.11          |
| (1,43)  | 1:16:A:ASP:H   | 1:17:A:SER:HA  | 13       | 0.11          |
| (1,692) | 1:35:A:CYS:SG  | 1:48:A:CYS:CB  | 10       | 0.1           |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,692) | 1:35:A:CYS:SG   | 1:48:A:CYS:CB  | 11       | 0.1           |
| (1,644) | 1:15:A:ASN:HB2  | 1:19:A:LEU:HB3 | 16       | 0.1           |
| (1,559) | 1:54:A:SER:HA   | 1:54:A:SER:HB2 | 14       | 0.1           |
| (1,554) | 1:19:A:LEU:HD11 | 1:20:A:ALA:HA  | 14       | 0.1           |
| (1,554) | 1:19:A:LEU:HD12 | 1:20:A:ALA:HA  | 14       | 0.1           |
| (1,554) | 1:19:A:LEU:HD13 | 1:20:A:ALA:HA  | 14       | 0.1           |
| (1,547) | 1:53:A:ASP:HA   | 1:54:A:SER:HA  | 13       | 0.1           |
| (1,547) | 1:53:A:ASP:HA   | 1:54:A:SER:HA  | 16       | 0.1           |
| (1,541) | 1:6:A:TYR:HA    | 1:17:A:SER:HB2 | 11       | 0.1           |
| (1,488) | 1:7:A:THR:HG21  | 1:11:A:CYS:H   | 15       | 0.1           |
| (1,488) | 1:7:A:THR:HG22  | 1:11:A:CYS:H   | 15       | 0.1           |
| (1,488) | 1:7:A:THR:HG23  | 1:11:A:CYS:H   | 15       | 0.1           |
| (1,360) | 1:22:A:ASP:HB2  | 1:23:A:THR:H   | 18       | 0.1           |
| (1,318) | 1:14:A:LYS:HE3  | 1:15:A:ASN:HB2 | 10       | 0.1           |
| (1,155) | 1:41:A:SER:HA   | 1:42:A:PHE:HB3 | 5        | 0.1           |
| (1,155) | 1:41:A:SER:HA   | 1:42:A:PHE:HB3 | 9        | 0.1           |
| (1,155) | 1:41:A:SER:HA   | 1:42:A:PHE:HB3 | 16       | 0.1           |
| (1,142) | 1:25:A:SER:H    | 1:26:A:GLY:H   | 6        | 0.1           |
| (1,109) | 1:38:A:GLN:HB2  | 1:40:A:PHE:HD1 | 18       | 0.1           |
| (1,109) | 1:38:A:GLN:HB2  | 1:40:A:PHE:HD2 | 18       | 0.1           |
| (1,109) | 1:38:A:GLN:HB3  | 1:40:A:PHE:HD1 | 18       | 0.1           |
| (1,109) | 1:38:A:GLN:HB3  | 1:40:A:PHE:HD2 | 18       | 0.1           |
| (1,80)  | 1:35:A:CYS:H    | 1:35:A:CYS:HB2 | 9        | 0.1           |
| (1,80)  | 1:35:A:CYS:H    | 1:35:A:CYS:HB2 | 12       | 0.1           |
| (1,80)  | 1:35:A:CYS:H    | 1:35:A:CYS:HB2 | 13       | 0.1           |
| (1,50)  | 1:25:A:SER:HA   | 1:52:A:ALA:H   | 13       | 0.1           |

## 10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found