



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 07:45 AM UTC

PDB ID : 6LCI / pdb\_00006lci  
BMRB ID : 36300  
Title : Solution structure of mdaA-1 domain  
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Deposited on : 2019-11-19

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

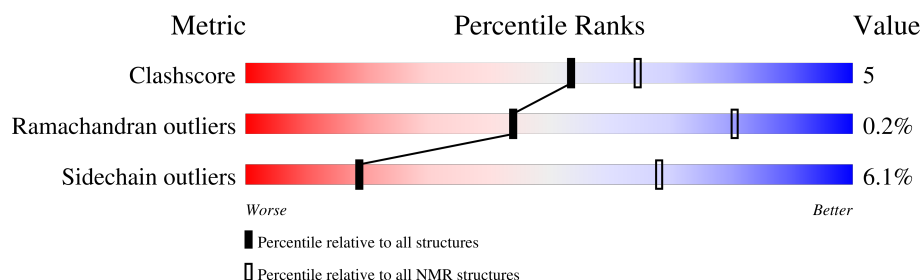
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 79%.

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     | 206    |                  |

## 2 Ensemble composition and analysis

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

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

| Well-defined (core) protein residues |                                                            |                   |              |
|--------------------------------------|------------------------------------------------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total)                                      | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:10-A:11, A:16-A:91,<br>A:101-A:126, A:133-A:160<br>(132) | 0.44              | 20           |

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

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

The models can be grouped into 2 clusters and 9 single-model clusters were found.

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

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

There is only 1 type of molecule in this entry. The entry contains 2589 atoms, of which 1292 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called mdaA-1.

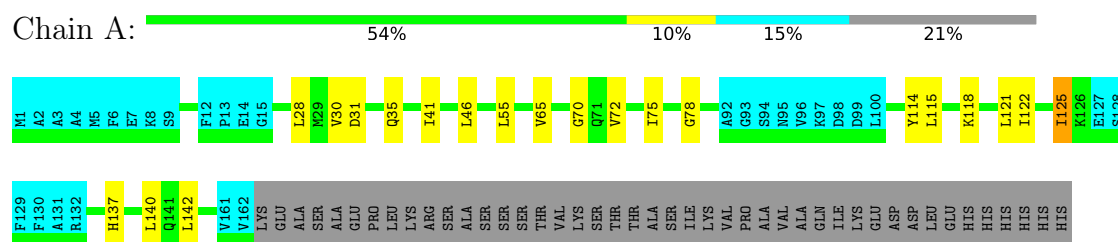
| Mol | Chain | Residues | Atoms |     |      |     |     |   | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 1   | A     | 162      | Total | C   | H    | N   | O   | S | 0     |
|     |       |          | 2589  | 830 | 1292 | 227 | 236 | 4 |       |

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

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

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

- Molecule 1: mdaA-1

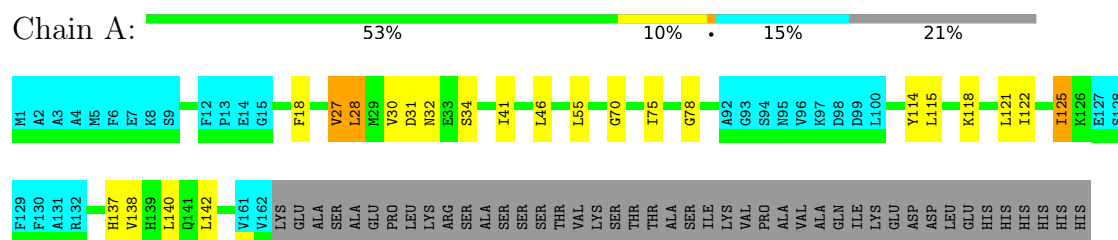


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

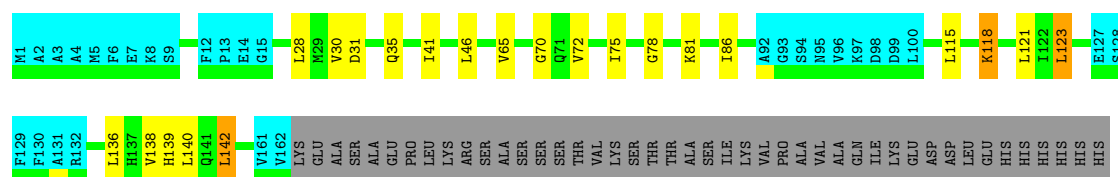
- Molecule 1: mdaA-1



#### 4.2.2 Score per residue for model 2

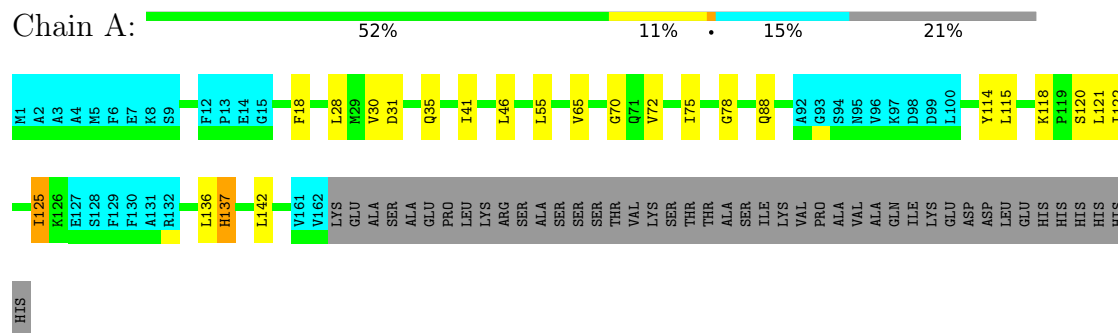
- Molecule 1: mdaA-1





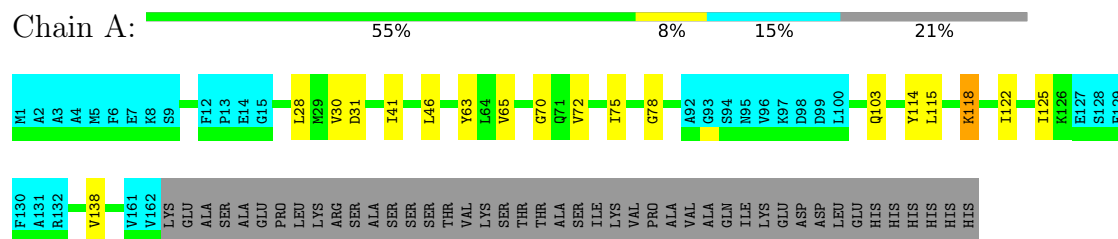
### 4.2.3 Score per residue for model 3

- Molecule 1: mdaA-1



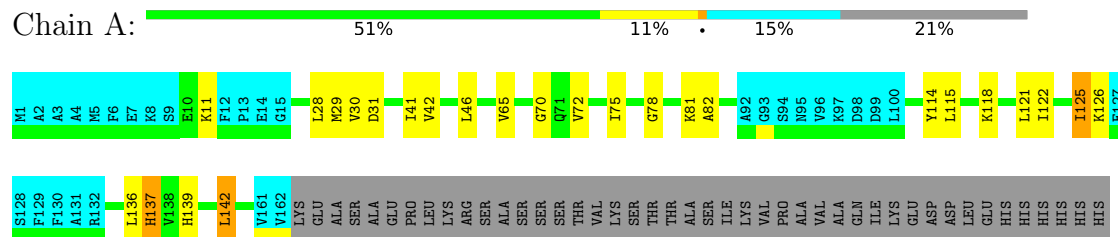
### 4.2.4 Score per residue for model 4

- Molecule 1: mdaA-1



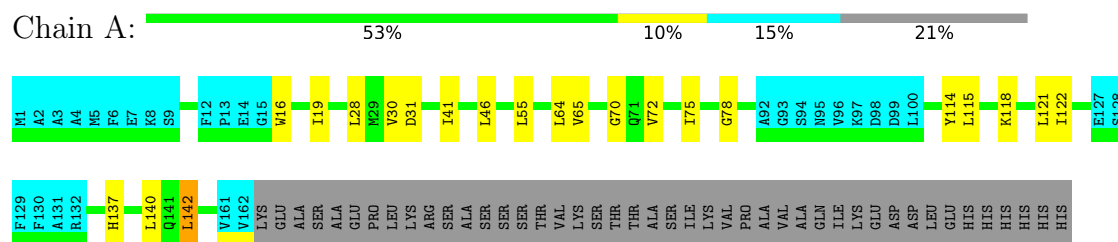
### 4.2.5 Score per residue for model 5

- Molecule 1: mdaA-1



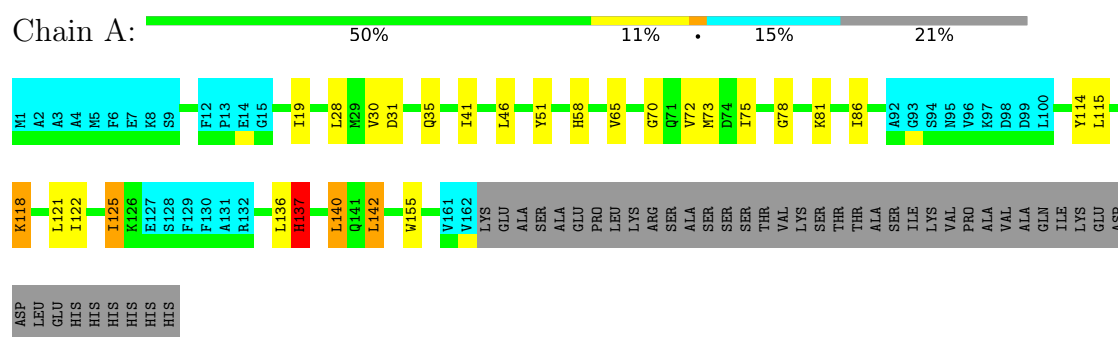
### 4.2.6 Score per residue for model 6

- Molecule 1: mdaA-1



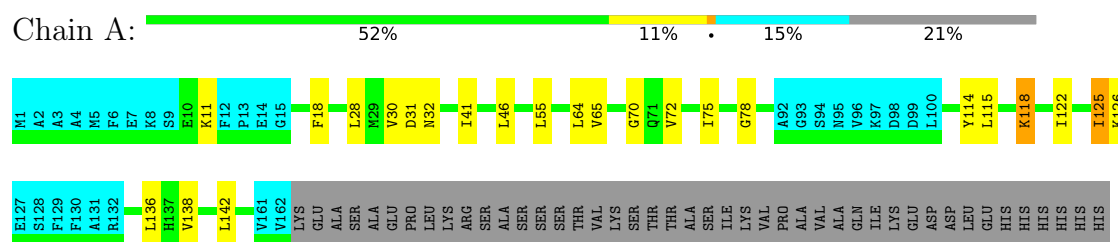
### 4.2.7 Score per residue for model 7

- Molecule 1: mdaA-1



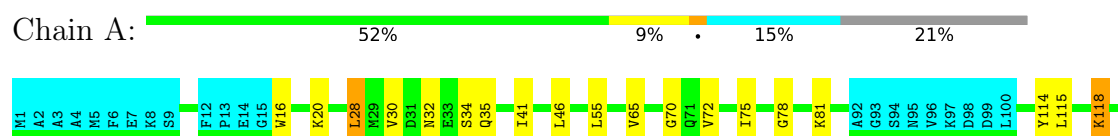
### 4.2.8 Score per residue for model 8

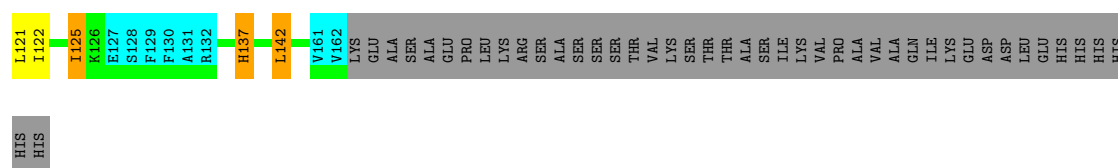
- Molecule 1: mdaA-1



### 4.2.9 Score per residue for model 9

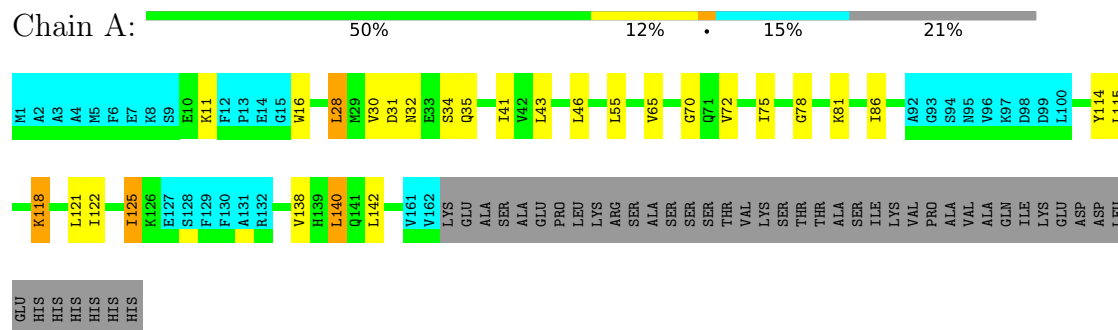
- Molecule 1: mdaA-1





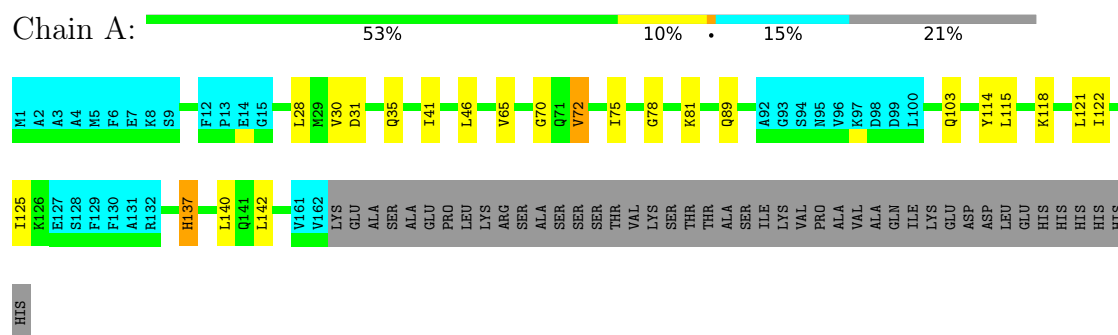
#### 4.2.10 Score per residue for model 10

- Molecule 1: mdaA-1



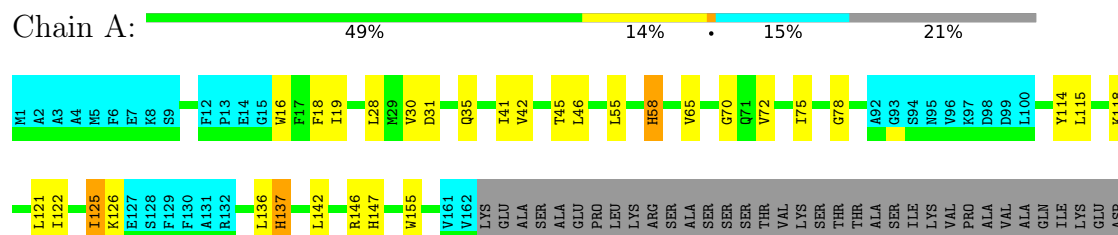
#### 4.2.11 Score per residue for model 11

- Molecule 1: mdaA-1



#### 4.2.12 Score per residue for model 12

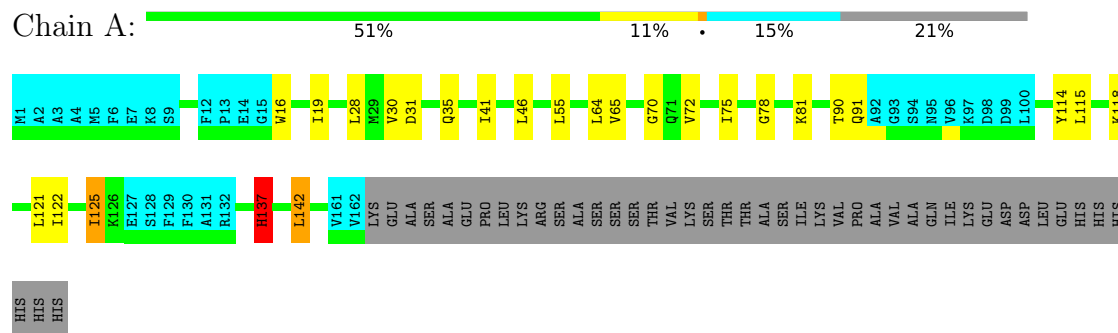
- Molecule 1: mdaA-1



ASP  
LEU  
GLU  
HIS  
HIS  
HIS  
HIS  
HIS

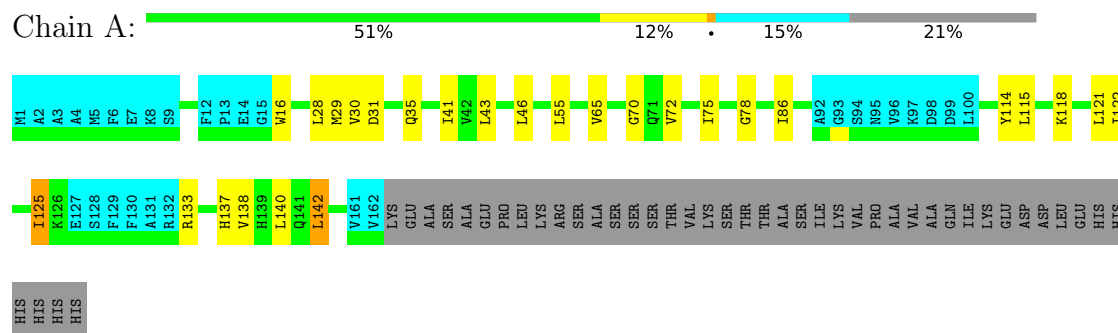
#### 4.2.13 Score per residue for model 13

- Molecule 1: mdaA-1



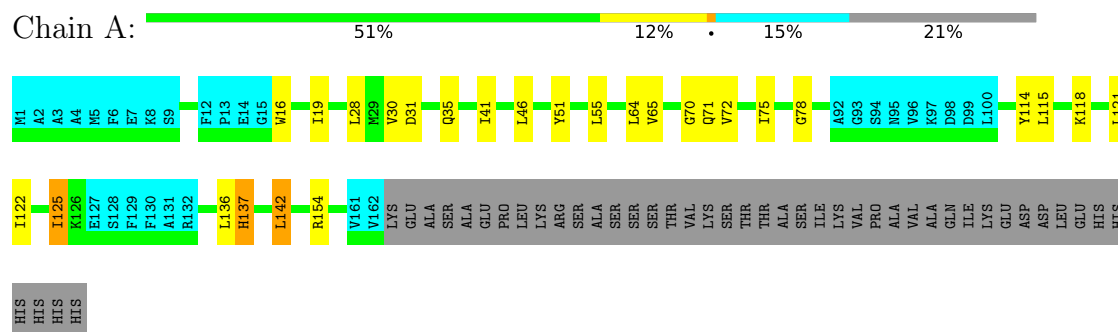
#### 4.2.14 Score per residue for model 14

- Molecule 1: mdaA-1



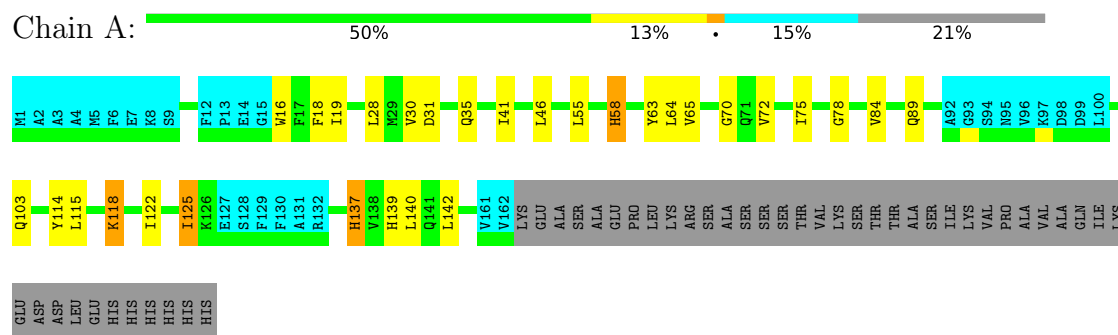
#### 4.2.15 Score per residue for model 15

- Molecule 1: mdaA-1



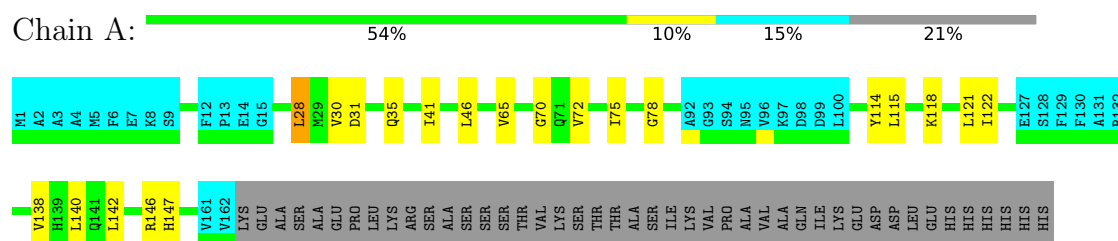
#### 4.2.16 Score per residue for model 16

- Molecule 1: mdaA-1



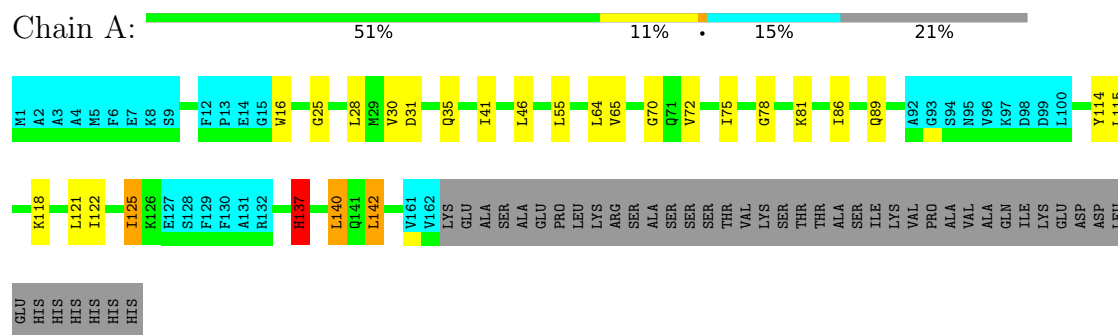
#### 4.2.17 Score per residue for model 17

- Molecule 1: mdaA-1



#### 4.2.18 Score per residue for model 18

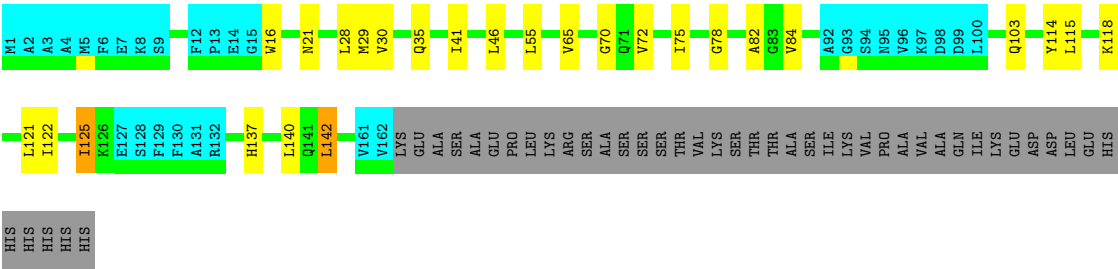
- Molecule 1: mdaA-1



#### 4.2.19 Score per residue for model 19

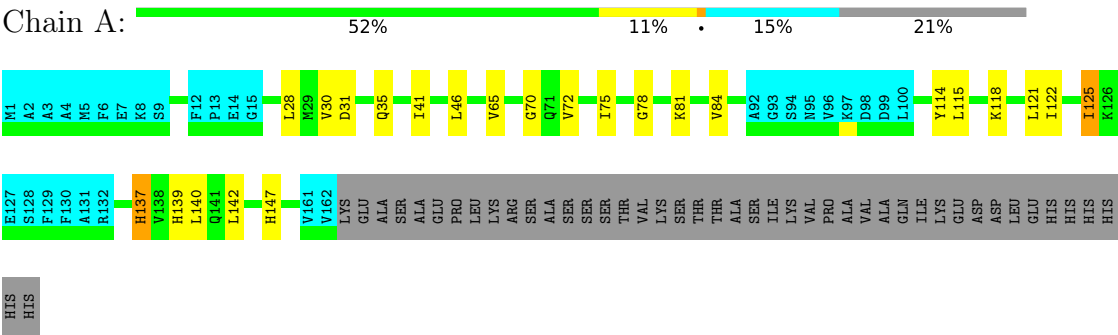
- Molecule 1: mdaA-1





4.2.20 Score per residue for model 20 (medoid)

• Molecule 1: mdaA-1



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| X-PLOR NIH    | structure calculation |         |
| X-PLOR NIH    | refinement            |         |

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

| Chemical shift file(s)                       | working_cs.cif |
|----------------------------------------------|----------------|
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 1745           |
| Number of shifts mapped to atoms             | 1745           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 79%            |

## 6 Model quality [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |                       | Bond angles |                       |
|-----|-------|--------------|-----------------------|-------------|-----------------------|
|     |       | RMSZ         | #Z>5                  | RMSZ        | #Z>5                  |
| 1   | A     | 1.16±0.00    | 0±0/1097 ( 0.0± 0.0%) | 1.23±0.01   | 3±1/1483 ( 0.2± 0.1%) |
| All | All   | 1.16         | 0/21940 ( 0.0%)       | 1.23        | 61/29660 ( 0.2%)      |

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|------------|-------|-------------|----------|--------|-------|
|     |       |     |      |            |       |             |          | Worst  | Total |
| 1   | A     | 78  | GLY  | N-CA-C     | -7.35 | 105.65      | 115.21   | 5      | 20    |
| 1   | A     | 70  | GLY  | N-CA-C     | -7.20 | 105.78      | 115.36   | 1      | 20    |
| 1   | A     | 35  | GLN  | N-CA-C     | -5.61 | 106.10      | 113.17   | 13     | 15    |
| 1   | A     | 25  | GLY  | N-CA-C     | -5.45 | 107.73      | 115.30   | 18     | 1     |
| 1   | A     | 133 | ARG  | N-CA-C     | -5.29 | 106.66      | 113.01   | 14     | 1     |
| 1   | A     | 120 | SER  | N-CA-C     | -5.11 | 107.05      | 113.28   | 3      | 1     |
| 1   | A     | 137 | HIS  | ND1-CG-CD2 | 5.05  | 111.15      | 106.10   | 7      | 3     |

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     | 1070  | 1074     | 1074     | 11±2    |
| All | All   | 21400 | 21480    | 21480    | 221     |

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 5.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:65:VAL:HG22  | 1:A:72:VAL:HG12  | 0.84     | 1.48        | 18     | 17    |
| 1:A:28:LEU:HD23  | 1:A:41:ILE:HG21  | 0.79     | 1.55        | 3      | 17    |
| 1:A:86:ILE:HD11  | 1:A:140:LEU:HD13 | 0.72     | 1.61        | 7      | 5     |
| 1:A:125:ILE:HD13 | 1:A:136:LEU:HD13 | 0.69     | 1.63        | 7      | 4     |
| 1:A:121:LEU:HD13 | 1:A:140:LEU:HD13 | 0.60     | 1.72        | 11     | 1     |
| 1:A:114:TYR:HB3  | 1:A:122:ILE:HG22 | 0.59     | 1.72        | 10     | 19    |
| 1:A:29:MET:HE2   | 1:A:30:VAL:O     | 0.58     | 1.98        | 14     | 3     |
| 1:A:84:VAL:CG1   | 1:A:140:LEU:HD12 | 0.58     | 2.29        | 16     | 2     |
| 1:A:121:LEU:HD23 | 1:A:140:LEU:HD13 | 0.56     | 1.76        | 19     | 1     |
| 1:A:28:LEU:HD12  | 1:A:41:ILE:HG21  | 0.56     | 1.75        | 5      | 3     |
| 1:A:19:ILE:HD11  | 1:A:64:LEU:HD13  | 0.54     | 1.79        | 15     | 1     |
| 1:A:30:VAL:HG12  | 1:A:31:ASP:H     | 0.54     | 1.63        | 8      | 3     |
| 1:A:65:VAL:HG22  | 1:A:72:VAL:CG1   | 0.53     | 2.34        | 5      | 10    |
| 1:A:72:VAL:HG21  | 1:A:103:GLN:NE2  | 0.53     | 2.19        | 16     | 2     |
| 1:A:58:HIS:CD2   | 1:A:58:HIS:O     | 0.52     | 2.62        | 16     | 3     |
| 1:A:121:LEU:HD12 | 1:A:140:LEU:HG   | 0.52     | 1.82        | 2      | 1     |
| 1:A:115:LEU:HD12 | 1:A:118:LYS:HB2  | 0.52     | 1.82        | 4      | 15    |
| 1:A:30:VAL:HG12  | 1:A:31:ASP:N     | 0.52     | 2.19        | 8      | 16    |
| 1:A:82:ALA:HB2   | 1:A:142:LEU:HD13 | 0.51     | 1.81        | 5      | 2     |
| 1:A:30:VAL:HG11  | 1:A:34:SER:H     | 0.51     | 1.65        | 10     | 3     |
| 1:A:18:PHE:CZ    | 1:A:55:LEU:HD21  | 0.50     | 2.41        | 3      | 5     |
| 1:A:16:TRP:HB3   | 1:A:55:LEU:HD22  | 0.50     | 1.82        | 12     | 10    |
| 1:A:121:LEU:HD12 | 1:A:140:LEU:HB3  | 0.50     | 1.83        | 20     | 1     |
| 1:A:121:LEU:HD23 | 1:A:142:LEU:CD1  | 0.50     | 2.37        | 6      | 4     |
| 1:A:125:ILE:HG22 | 1:A:137:HIS:O    | 0.50     | 2.06        | 12     | 14    |
| 1:A:121:LEU:HD23 | 1:A:142:LEU:HD12 | 0.50     | 1.84        | 11     | 9     |
| 1:A:65:VAL:HG22  | 1:A:72:VAL:HG22  | 0.49     | 1.84        | 13     | 2     |
| 1:A:121:LEU:HD23 | 1:A:140:LEU:HB3  | 0.49     | 1.84        | 17     | 2     |
| 1:A:84:VAL:HB    | 1:A:140:LEU:HD12 | 0.49     | 1.85        | 19     | 1     |
| 1:A:31:ASP:HA    | 1:A:42:VAL:HG22  | 0.48     | 1.84        | 5      | 2     |
| 1:A:43:LEU:HD11  | 1:A:125:ILE:HG21 | 0.46     | 1.86        | 14     | 2     |
| 1:A:30:VAL:HG22  | 1:A:31:ASP:H     | 0.46     | 1.70        | 10     | 2     |
| 1:A:19:ILE:HD11  | 1:A:64:LEU:CD2   | 0.46     | 2.40        | 6      | 3     |
| 1:A:19:ILE:HG22  | 1:A:155:TRP:CE3  | 0.45     | 2.46        | 7      | 2     |
| 1:A:121:LEU:CD2  | 1:A:140:LEU:HD13 | 0.45     | 2.41        | 19     | 1     |
| 1:A:123:LEU:H    | 1:A:123:LEU:HD22 | 0.45     | 1.70        | 2      | 1     |
| 1:A:146:ARG:HG3  | 1:A:147:HIS:CD2  | 0.45     | 2.47        | 12     | 2     |
| 1:A:28:LEU:HD11  | 1:A:73:MET:HE2   | 0.44     | 1.89        | 7      | 1     |
| 1:A:115:LEU:HB2  | 1:A:118:LYS:H    | 0.44     | 1.73        | 14     | 15    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:28:LEU:HD23  | 1:A:41:ILE:CG2   | 0.43     | 2.40        | 14     | 1     |
| 1:A:121:LEU:HD12 | 1:A:140:LEU:CG   | 0.43     | 2.44        | 2      | 1     |
| 1:A:126:LYS:O    | 1:A:136:LEU:HD22 | 0.42     | 2.14        | 5      | 3     |
| 1:A:63:TYR:CD2   | 1:A:103:GLN:HB2  | 0.41     | 2.50        | 4      | 2     |
| 1:A:121:LEU:HD23 | 1:A:140:LEU:CB   | 0.41     | 2.45        | 17     | 1     |
| 1:A:121:LEU:HD22 | 1:A:140:LEU:HB3  | 0.41     | 1.93        | 11     | 2     |
| 1:A:121:LEU:HD13 | 1:A:142:LEU:HD12 | 0.41     | 1.93        | 2      | 1     |
| 1:A:90:THR:HG22  | 1:A:91:GLN:N     | 0.41     | 2.31        | 13     | 1     |
| 1:A:18:PHE:CE1   | 1:A:55:LEU:HD21  | 0.41     | 2.51        | 12     | 1     |
| 1:A:27:VAL:CG2   | 1:A:28:LEU:N     | 0.40     | 2.84        | 1      | 1     |

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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

| Mol | Chain | Analysed        | Favoured      | Allowed    | Outliers   | Percentiles |    |
|-----|-------|-----------------|---------------|------------|------------|-------------|----|
| 1   | A     | 132/206 (64%)   | 130±1 (98±1%) | 2±1 (2±1%) | 0±0 (0±0%) | 44          | 80 |
| All | All   | 2640/4120 (64%) | 2592 (98%)    | 44 (2%)    | 4 (0%)     | 44          | 80 |

All 1 unique Ramachandran outliers are listed below.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 32  | ASN  | 4              |

### 6.3.2 Protein sidechains ⓘ

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

| Mol | Chain | Analysed        | Rotameric     | Outliers   | Percentiles |    |
|-----|-------|-----------------|---------------|------------|-------------|----|
| 1   | A     | 117/178 (66%)   | 110±2 (94±1%) | 7±2 (6±1%) | 19          | 68 |
| All | All   | 2340/3560 (66%) | 2197 (94%)    | 143 (6%)   | 19          | 68 |

All 28 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     | 46  | LEU  | 20             |
| 1   | A     | 75  | ILE  | 20             |
| 1   | A     | 125 | ILE  | 16             |
| 1   | A     | 142 | LEU  | 15             |
| 1   | A     | 137 | HIS  | 12             |
| 1   | A     | 81  | LYS  | 9              |
| 1   | A     | 118 | LYS  | 8              |
| 1   | A     | 138 | VAL  | 7              |
| 1   | A     | 28  | LEU  | 4              |
| 1   | A     | 139 | HIS  | 4              |
| 1   | A     | 11  | LYS  | 3              |
| 1   | A     | 140 | LEU  | 3              |
| 1   | A     | 89  | GLN  | 3              |
| 1   | A     | 51  | TYR  | 2              |
| 1   | A     | 64  | LEU  | 2              |
| 1   | A     | 103 | GLN  | 2              |
| 1   | A     | 58  | HIS  | 2              |
| 1   | A     | 27  | VAL  | 1              |
| 1   | A     | 123 | LEU  | 1              |
| 1   | A     | 88  | GLN  | 1              |
| 1   | A     | 115 | LEU  | 1              |
| 1   | A     | 20  | LYS  | 1              |
| 1   | A     | 72  | VAL  | 1              |
| 1   | A     | 45  | THR  | 1              |
| 1   | A     | 71  | GLN  | 1              |
| 1   | A     | 154 | ARG  | 1              |
| 1   | A     | 21  | ASN  | 1              |
| 1   | A     | 147 | HIS  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 79% for the well-defined parts and 78% for the entire structure.

### 7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: `mdaA_cs.str`

#### 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                  | 1745 |
| Number of shifts mapped to atoms        | 1745 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 11   |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 161      | $0.38 \pm 0.12$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 147      | $0.01 \pm 0.09$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 0        | —                               | None (insufficient data)   |
| $^{15}\text{N}$        | 152      | $0.20 \pm 0.32$                 | None needed ( $< 0.5$ ppm) |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 79%, i.e. 1482 atoms were assigned a chemical shift out of a possible 1866. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | $^1\text{H}$   | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|----------------|----------------|-----------------|-----------------|
| Backbone  | 526/658 (80%)  | 268/268 (100%) | 132/264 (50%)   | 126/126 (100%)  |
| Sidechain | 876/1042 (84%) | 577/674 (86%)  | 282/322 (88%)   | 17/46 (37%)     |

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|          | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|-----------------|----------------|-----------------|-----------------|
| Aromatic | 80/166 (48%)    | 40/83 (48%)    | 37/75 (49%)     | 3/8 (38%)       |
| Overall  | 1482/1866 (79%) | 885/1025 (86%) | 451/661 (68%)   | 146/180 (81%)   |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 1745 atoms were assigned a chemical shift out of a possible 2249. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H  | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|-----------------|-----------------|-----------------|
| Backbone  | 638/808 (79%)   | 325/329 (99%)   | 161/324 (50%)   | 152/155 (98%)   |
| Sidechain | 1011/1235 (82%) | 664/800 (83%)   | 329/383 (86%)   | 18/52 (35%)     |
| Aromatic  | 96/206 (47%)    | 48/103 (47%)    | 45/95 (47%)     | 3/8 (38%)       |
| Overall   | 1745/2249 (78%) | 1037/1232 (84%) | 535/802 (67%)   | 173/215 (80%)   |

#### 7.1.4 Statistically unusual chemical shifts ⓘ

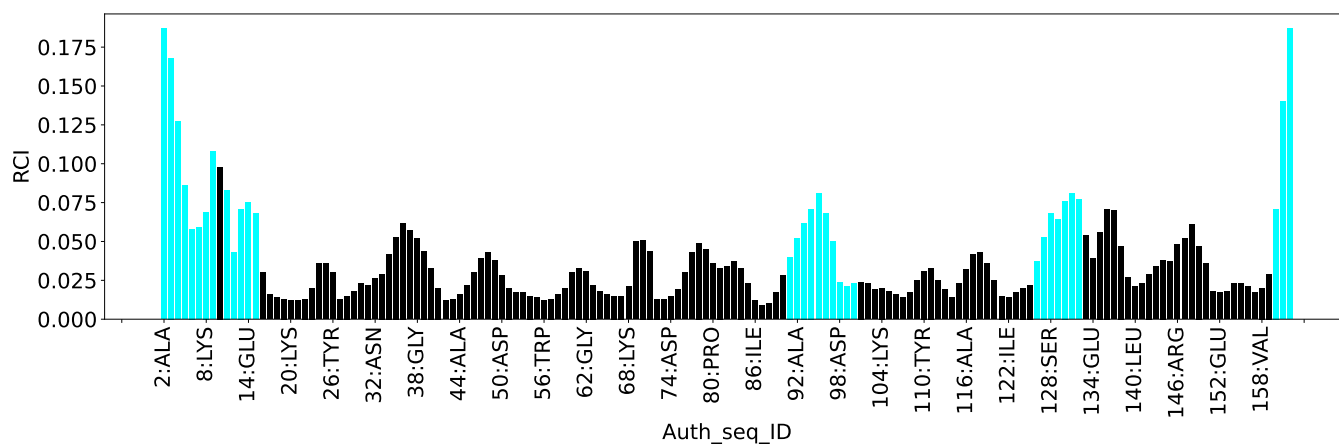
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 67  | LYS  | HD2  | -0.17      | 0.58 – 2.64         | -8.6    |
| 1       | A     | 66  | ASN  | HD21 | 3.38       | 4.94 – 9.72         | -8.3    |
| 1       | A     | 21  | ASN  | HD21 | 3.72       | 4.94 – 9.72         | -7.5    |
| 1       | A     | 67  | LYS  | HG2  | -0.45      | 0.13 – 2.61         | -7.3    |
| 1       | A     | 57  | ARG  | HD2  | 1.59       | 1.97 – 4.26         | -6.7    |
| 1       | A     | 57  | ARG  | HB2  | 0.16       | 0.52 – 3.08         | -6.4    |
| 1       | A     | 67  | LYS  | HB2  | 0.25       | 0.58 – 2.97         | -6.4    |
| 1       | A     | 13  | PRO  | HD2  | 1.62       | 1.93 – 5.38         | -5.9    |
| 1       | A     | 29  | MET  | CG   | 39.47      | 25.46 – 38.60       | 5.7     |
| 1       | A     | 67  | LYS  | HD3  | 0.49       | 0.54 – 2.65         | -5.3    |
| 1       | A     | 67  | LYS  | HE2  | 1.92       | 1.95 – 3.88         | -5.1    |

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

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                                | 1664  |
| Intra-residue ( $ i-j =0$ )                              | 452   |
| Sequential ( $ i-j =1$ )                                 | 572   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 180   |
| Long range ( $ i-j \geq 5$ )                             | 460   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 225   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 9.2   |
| Number of long range restraints per residue <sup>1</sup> | 2.2   |

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

### 8.2 Residual restraint violations

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

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

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

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|----------------------------------------|---------|
| 0.1-0.2 (Small)  | 30.4                                   | 0.2     |
| 0.2-0.5 (Medium) | 32.8                                   | 0.5     |
| >0.5 (Large)     | 0.8                                    | 0.81    |

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

Dihedral-angle violations less than 1° are not included in the calculation.

| Bins (°)           | Average number of violations per model | Max (°) |
|--------------------|----------------------------------------|---------|
| 1.0-10.0 (Small)   | 8.5                                    | 5.49    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

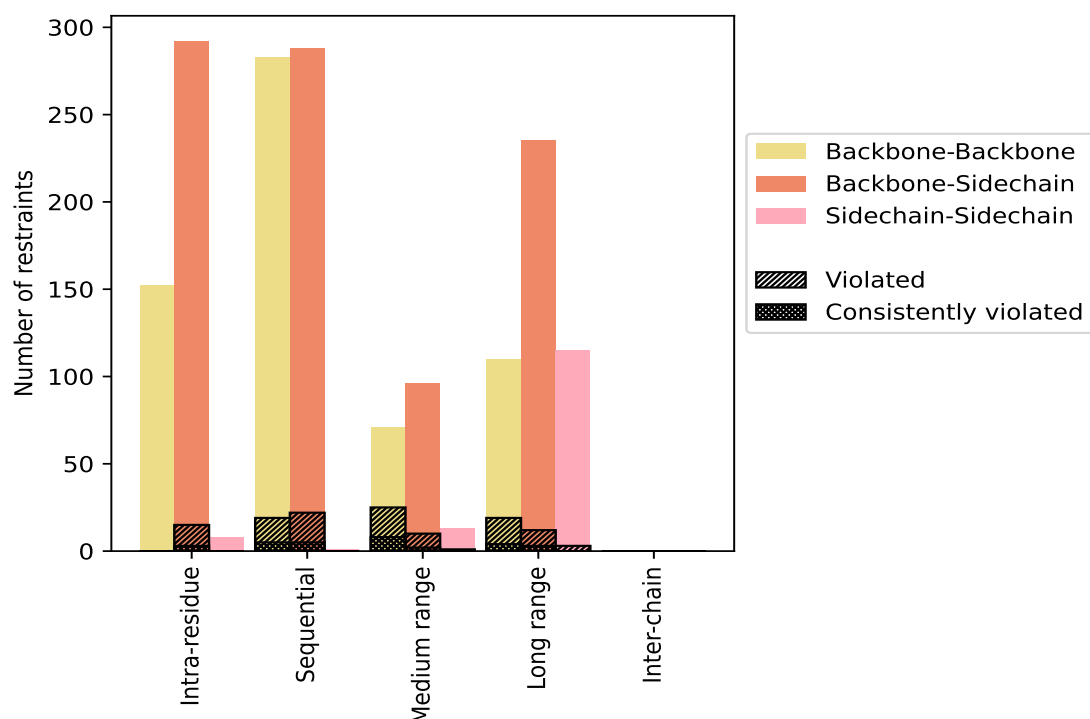
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                                              | Count       | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|-----------------------------------------------------------------------------|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                                                             |             |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>452</b>  | <b>27.2</b>    | <b>15</b>             | <b>3.3</b>     | <b>0.9</b>     | <b>3</b>                           | <b>0.7</b>     | <b>0.2</b>     |
| Backbone-Backbone                                                           | 152         | 9.1            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 292         | 17.5           | 15                    | 5.1            | 0.9            | 3                                  | 1.0            | 0.2            |
| Sidechain-Sidechain                                                         | 8           | 0.5            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>572</b>  | <b>34.4</b>    | <b>41</b>             | <b>7.2</b>     | <b>2.5</b>     | <b>10</b>                          | <b>1.7</b>     | <b>0.6</b>     |
| Backbone-Backbone                                                           | 283         | 17.0           | 19                    | 6.7            | 1.1            | 5                                  | 1.8            | 0.3            |
| Backbone-Sidechain                                                          | 288         | 17.3           | 22                    | 7.6            | 1.3            | 5                                  | 1.7            | 0.3            |
| Sidechain-Sidechain                                                         | 1           | 0.1            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>180</b>  | <b>10.8</b>    | <b>36</b>             | <b>20.0</b>    | <b>2.2</b>     | <b>10</b>                          | <b>5.6</b>     | <b>0.6</b>     |
| Backbone-Backbone                                                           | 71          | 4.3            | 25                    | 35.2           | 1.5            | 8                                  | 11.3           | 0.5            |
| Backbone-Sidechain                                                          | 96          | 5.8            | 10                    | 10.4           | 0.6            | 2                                  | 2.1            | 0.1            |
| Sidechain-Sidechain                                                         | 13          | 0.8            | 1                     | 7.7            | 0.1            | 0                                  | 0.0            | 0.0            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>460</b>  | <b>27.6</b>    | <b>34</b>             | <b>7.4</b>     | <b>2.0</b>     | <b>7</b>                           | <b>1.5</b>     | <b>0.4</b>     |
| Backbone-Backbone                                                           | 110         | 6.6            | 19                    | 17.3           | 1.1            | 4                                  | 3.6            | 0.2            |
| Backbone-Sidechain                                                          | 235         | 14.1           | 12                    | 5.1            | 0.7            | 3                                  | 1.3            | 0.2            |
| Sidechain-Sidechain                                                         | 115         | 6.9            | 3                     | 2.6            | 0.2            | 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>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>                                                                | <b>1664</b> | <b>100.0</b>   | <b>126</b>            | <b>7.6</b>     | <b>7.6</b>     | <b>30</b>                          | <b>1.8</b>     | <b>1.8</b>     |
| Backbone-Backbone                                                           | 616         | 37.0           | 63                    | 10.2           | 3.8            | 17                                 | 2.8            | 1.0            |
| Backbone-Sidechain                                                          | 911         | 54.7           | 59                    | 6.5            | 3.5            | 13                                 | 1.4            | 0.8            |
| Sidechain-Sidechain                                                         | 137         | 8.2            | 4                     | 2.9            | 0.2            | 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 disulfied bonds are counted in their appropriate category on the x-axis

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 7                    | 22              | 25              | 20              | 0               | 74    | 0.22     | 0.51    | 0.09                | 0.2        |
| 2        | 10                   | 20              | 20              | 16              | 0               | 66    | 0.22     | 0.46    | 0.1                 | 0.2        |
| 3        | 7                    | 20              | 22              | 16              | 0               | 65    | 0.24     | 0.46    | 0.1                 | 0.24       |
| 4        | 7                    | 19              | 22              | 16              | 0               | 64    | 0.24     | 0.75    | 0.12                | 0.21       |
| 5        | 6                    | 22              | 22              | 16              | 0               | 66    | 0.23     | 0.7     | 0.12                | 0.22       |
| 6        | 8                    | 18              | 21              | 18              | 0               | 65    | 0.24     | 0.5     | 0.11                | 0.21       |
| 7        | 4                    | 21              | 23              | 17              | 0               | 65    | 0.22     | 0.44    | 0.1                 | 0.19       |
| 8        | 6                    | 19              | 23              | 20              | 0               | 68    | 0.23     | 0.59    | 0.1                 | 0.22       |
| 9        | 4                    | 22              | 24              | 19              | 0               | 69    | 0.23     | 0.78    | 0.12                | 0.21       |
| 10       | 6                    | 19              | 26              | 17              | 0               | 68    | 0.23     | 0.78    | 0.12                | 0.21       |

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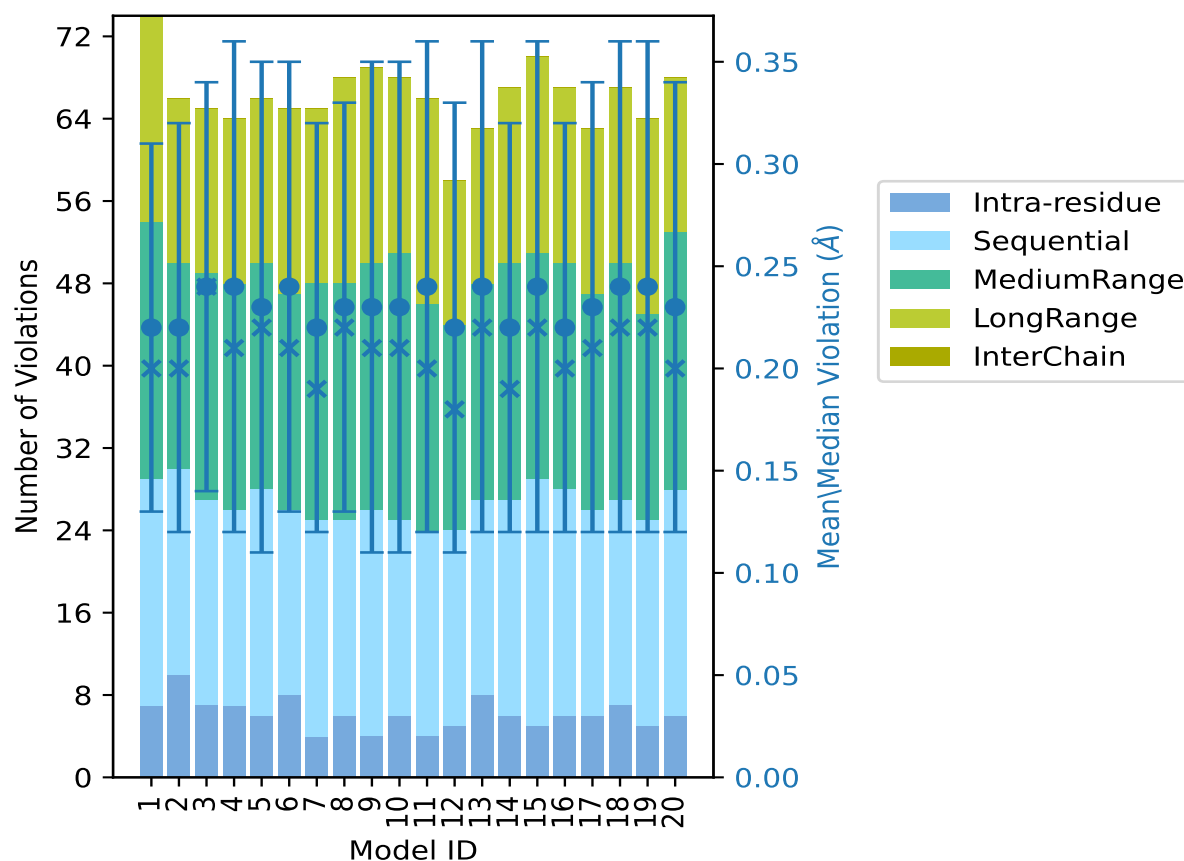
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 4                    | 20              | 22              | 20              | 0               | 66    | 0.24     | 0.76    | 0.12                | 0.2        |
| 12       | 5                    | 19              | 20              | 14              | 0               | 58    | 0.22     | 0.51    | 0.11                | 0.18       |
| 13       | 8                    | 19              | 21              | 15              | 0               | 63    | 0.24     | 0.7     | 0.12                | 0.22       |
| 14       | 6                    | 21              | 23              | 17              | 0               | 67    | 0.22     | 0.45    | 0.1                 | 0.19       |
| 15       | 5                    | 24              | 22              | 19              | 0               | 70    | 0.24     | 0.81    | 0.12                | 0.22       |
| 16       | 6                    | 22              | 22              | 17              | 0               | 67    | 0.22     | 0.46    | 0.1                 | 0.2        |
| 17       | 6                    | 20              | 21              | 16              | 0               | 63    | 0.23     | 0.66    | 0.11                | 0.21       |
| 18       | 7                    | 20              | 23              | 17              | 0               | 67    | 0.24     | 0.76    | 0.12                | 0.22       |
| 19       | 5                    | 20              | 20              | 19              | 0               | 64    | 0.24     | 0.65    | 0.12                | 0.22       |
| 20       | 6                    | 22              | 25              | 15              | 0               | 68    | 0.23     | 0.62    | 0.11                | 0.2        |

<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

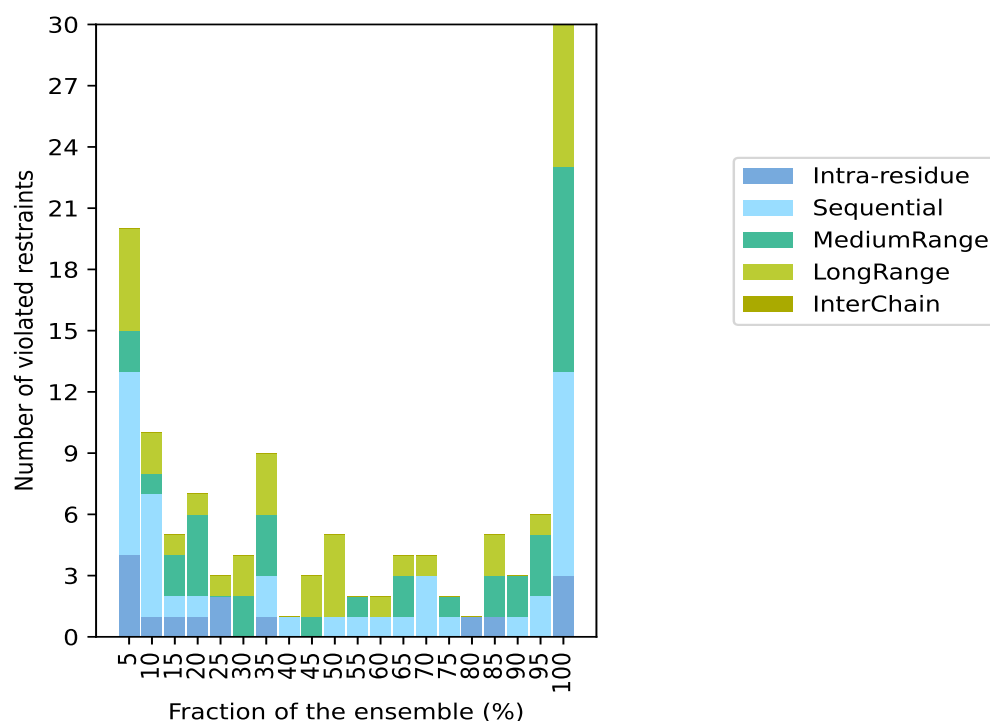
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1538(IR:437, SQ:531, MR:144, LR:426, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 4                             | 9               | 2               | 5               | 0               | 20    | 1                        | 5.0   |
| 1                             | 6               | 1               | 2               | 0               | 10    | 2                        | 10.0  |
| 1                             | 1               | 2               | 1               | 0               | 5     | 3                        | 15.0  |
| 1                             | 1               | 4               | 1               | 0               | 7     | 4                        | 20.0  |
| 2                             | 0               | 0               | 1               | 0               | 3     | 5                        | 25.0  |
| 0                             | 0               | 2               | 2               | 0               | 4     | 6                        | 30.0  |
| 1                             | 2               | 3               | 3               | 0               | 9     | 7                        | 35.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 8                        | 40.0  |
| 0                             | 0               | 1               | 2               | 0               | 3     | 9                        | 45.0  |
| 0                             | 1               | 0               | 4               | 0               | 5     | 10                       | 50.0  |
| 0                             | 1               | 1               | 0               | 0               | 2     | 11                       | 55.0  |
| 0                             | 1               | 0               | 1               | 0               | 2     | 12                       | 60.0  |
| 0                             | 1               | 2               | 1               | 0               | 4     | 13                       | 65.0  |
| 0                             | 3               | 0               | 1               | 0               | 4     | 14                       | 70.0  |
| 0                             | 1               | 1               | 0               | 0               | 2     | 15                       | 75.0  |
| 1                             | 0               | 0               | 0               | 0               | 1     | 16                       | 80.0  |
| 1                             | 0               | 2               | 2               | 0               | 5     | 17                       | 85.0  |
| 0                             | 1               | 2               | 0               | 0               | 3     | 18                       | 90.0  |
| 0                             | 2               | 3               | 1               | 0               | 6     | 19                       | 95.0  |
| 3                             | 10              | 10              | 7               | 0               | 30    | 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

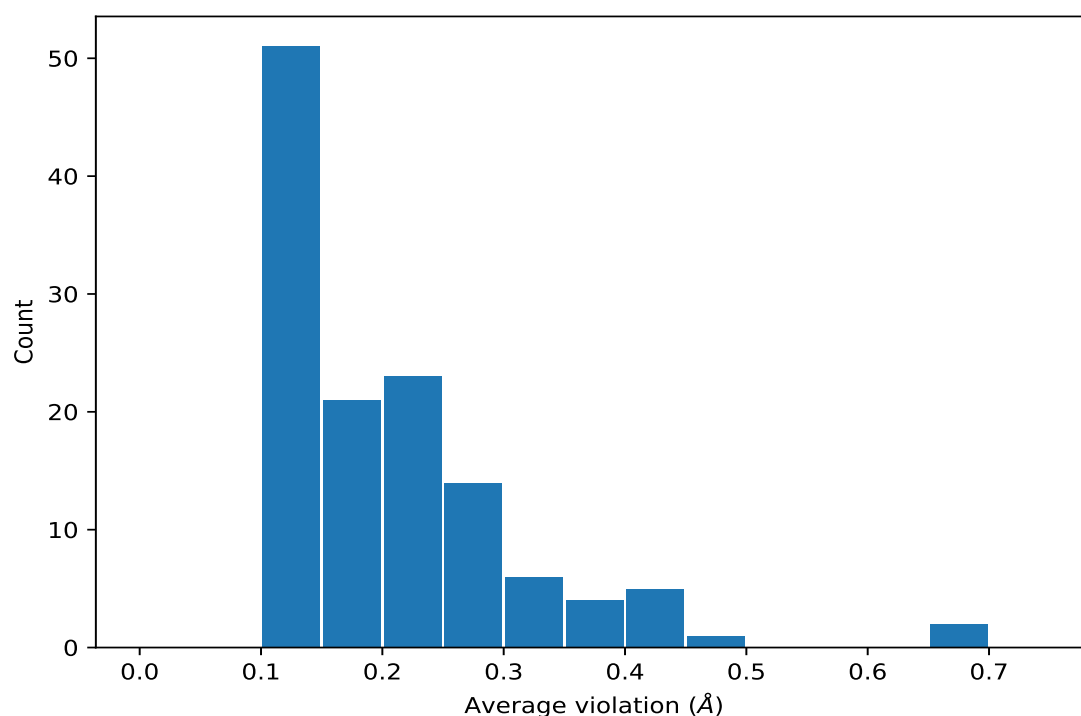
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|----------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,1335) | 1:134:A:GLU:H   | 1:135:A:GLY:H  | 20                  | 0.46     | 0.03                | 0.46       |
| (1,587)  | 1:56:A:TRP:HE3  | 1:56:A:TRP:H   | 20                  | 0.44     | 0.02                | 0.45       |
| (1,1008) | 1:99:A:ASP:HA   | 1:100:A:LEU:H  | 20                  | 0.42     | 0.02                | 0.42       |
| (1,601)  | 1:57:A:ARG:H    | 1:64:A:LEU:HA  | 20                  | 0.38     | 0.05                | 0.38       |
| (1,112)  | 1:17:A:PHE:H    | 1:18:A:PHE:HE1 | 20                  | 0.38     | 0.02                | 0.38       |
| (1,1357) | 1:138:A:VAL:HB  | 1:139:A:HIS:H  | 20                  | 0.38     | 0.04                | 0.37       |
| (1,851)  | 1:81:A:LYS:H    | 1:84:A:VAL:H   | 20                  | 0.37     | 0.05                | 0.36       |
| (1,812)  | 1:77:A:LYS:HA   | 1:79:A:THR:H   | 20                  | 0.35     | 0.01                | 0.35       |
| (1,1162) | 1:115:A:LEU:HG  | 1:118:A:LYS:H  | 20                  | 0.33     | 0.03                | 0.34       |
| (1,549)  | 1:53:A:SER:H    | 1:55:A:LEU:H   | 20                  | 0.33     | 0.02                | 0.34       |
| (1,720)  | 1:68:A:LYS:H    | 1:70:A:GLY:H   | 20                  | 0.33     | 0.03                | 0.33       |
| (1,1656) | 1:137:A:HIS:HE1 | 1:126:A:LYS:H  | 20                  | 0.31     | 0.05                | 0.32       |
| (1,728)  | 1:69:A:SER:H    | 1:71:A:GLN:H   | 20                  | 0.31     | 0.11                | 0.36       |
| (1,696)  | 1:66:A:ASN:H    | 1:70:A:GLY:H   | 20                  | 0.28     | 0.06                | 0.28       |
| (1,116)  | 1:17:A:PHE:H    | 1:56:A:TRP:HD1 | 20                  | 0.27     | 0.05                | 0.27       |
| (1,1018) | 1:100:A:LEU:HA  | 1:101:A:ASN:H  | 20                  | 0.27     | 0.02                | 0.26       |

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| Key      | Atom-1          | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,1525) | 1:158:A:VAL:HB  | 1:159:A:LEU:H  | 20                  | 0.26     | 0.02                | 0.26       |
| (1,1073) | 1:106:A:GLY:H   | 1:114:A:TYR:H  | 20                  | 0.25     | 0.04                | 0.27       |
| (1,1402) | 1:144:A:ASP:H   | 1:145:A:LYS:H  | 20                  | 0.25     | 0.06                | 0.24       |
| (1,1016) | 1:99:A:ASP:H    | 1:101:A:ASN:H  | 20                  | 0.25     | 0.04                | 0.25       |
| (1,1163) | 1:115:A:LEU:HG  | 1:120:A:SER:H  | 20                  | 0.24     | 0.03                | 0.25       |
| (1,225)  | 1:23:A:SER:H    | 1:25:A:GLY:H   | 20                  | 0.23     | 0.07                | 0.24       |
| (1,441)  | 1:43:A:LEU:HA   | 1:135:A:GLY:H  | 20                  | 0.22     | 0.03                | 0.22       |
| (1,1155) | 1:115:A:LEU:HB2 | 1:118:A:LYS:H  | 20                  | 0.21     | 0.04                | 0.22       |
| (1,1155) | 1:115:A:LEU:HB3 | 1:118:A:LYS:H  | 20                  | 0.21     | 0.04                | 0.22       |
| (1,783)  | 1:75:A:ILE:HB   | 1:76:A:ALA:H   | 20                  | 0.18     | 0.03                | 0.17       |
| (1,305)  | 1:29:A:MET:H    | 1:42:A:VAL:H   | 20                  | 0.16     | 0.03                | 0.16       |
| (1,98)   | 1:16:A:TRP:HD1  | 1:16:A:TRP:H   | 20                  | 0.16     | 0.03                | 0.16       |
| (1,483)  | 1:46:A:LEU:HG   | 1:46:A:LEU:H   | 20                  | 0.13     | 0.02                | 0.13       |
| (1,1160) | 1:115:A:LEU:HG  | 1:116:A:ALA:H  | 20                  | 0.13     | 0.02                | 0.13       |
| (1,711)  | 1:68:A:LYS:HA   | 1:69:A:SER:H   | 20                  | 0.12     | 0.01                | 0.12       |
| (1,357)  | 1:34:A:SER:HA   | 1:36:A:GLU:H   | 19                  | 0.28     | 0.06                | 0.29       |
| (1,1461) | 1:150:A:ARG:H   | 1:152:A:GLU:H  | 19                  | 0.23     | 0.05                | 0.25       |
| (1,1485) | 1:152:A:GLU:H   | 1:154:A:ARG:H  | 19                  | 0.23     | 0.04                | 0.23       |
| (1,927)  | 1:90:A:THR:HB   | 1:91:A:GLN:H   | 19                  | 0.21     | 0.07                | 0.19       |
| (1,1442) | 1:149:A:ASP:HA  | 1:150:A:ARG:H  | 19                  | 0.2      | 0.05                | 0.18       |
| (1,881)  | 1:84:A:VAL:H    | 1:140:A:LEU:H  | 19                  | 0.16     | 0.03                | 0.15       |
| (1,468)  | 1:45:A:THR:HB   | 1:46:A:LEU:H   | 18                  | 0.23     | 0.09                | 0.18       |
| (1,488)  | 1:47:A:ARG:HA   | 1:49:A:LYS:H   | 18                  | 0.19     | 0.08                | 0.15       |
| (1,1321) | 1:133:A:ARG:HA  | 1:136:A:LEU:H  | 18                  | 0.18     | 0.03                | 0.18       |
| (1,284)  | 1:28:A:LEU:HG   | 1:28:A:LEU:H   | 17                  | 0.25     | 0.03                | 0.25       |
| (1,623)  | 1:59:A:ASP:H    | 1:63:A:TYR:HD1 | 17                  | 0.23     | 0.11                | 0.21       |
| (1,1405) | 1:145:A:LYS:HA  | 1:147:A:HIS:H  | 17                  | 0.17     | 0.04                | 0.16       |
| (1,291)  | 1:29:A:MET:HA   | 1:56:A:TRP:HE1 | 17                  | 0.16     | 0.04                | 0.16       |
| (1,115)  | 1:17:A:PHE:H    | 1:56:A:TRP:HA  | 17                  | 0.15     | 0.03                | 0.15       |
| (1,992)  | 1:97:A:LYS:HG2  | 1:97:A:LYS:H   | 16                  | 0.14     | 0.01                | 0.14       |
| (1,992)  | 1:97:A:LYS:HG3  | 1:97:A:LYS:H   | 16                  | 0.14     | 0.01                | 0.14       |
| (1,1310) | 1:132:A:ARG:HA  | 1:134:A:GLU:H  | 15                  | 0.27     | 0.07                | 0.29       |
| (1,960)  | 1:95:A:ASN:HA   | 1:96:A:VAL:H   | 15                  | 0.22     | 0.05                | 0.22       |
| (1,253)  | 1:26:A:TYR:HE1  | 1:45:A:THR:H   | 14                  | 0.29     | 0.06                | 0.28       |
| (1,253)  | 1:26:A:TYR:HE2  | 1:45:A:THR:H   | 14                  | 0.29     | 0.06                | 0.28       |
| (1,647)  | 1:62:A:GLY:H    | 1:63:A:TYR:HD1 | 14                  | 0.15     | 0.03                | 0.14       |
| (1,570)  | 1:55:A:LEU:H    | 1:56:A:TRP:HE1 | 14                  | 0.14     | 0.03                | 0.14       |
| (1,214)  | 1:23:A:SER:HA   | 1:24:A:ASN:H   | 14                  | 0.11     | 0.01                | 0.11       |
| (1,1655) | 1:58:A:HIS:HE1  | 1:62:A:GLY:HA2 | 13                  | 0.68     | 0.13                | 0.7        |
| (1,1655) | 1:58:A:HIS:HE1  | 1:62:A:GLY:HA3 | 13                  | 0.68     | 0.13                | 0.7        |
| (1,1307) | 1:131:A:ALA:H   | 1:132:A:ARG:H  | 13                  | 0.4      | 0.06                | 0.4        |
| (1,608)  | 1:58:A:HIS:HA   | 1:65:A:VAL:H   | 13                  | 0.17     | 0.03                | 0.16       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1639) | 1:115:A:LEU:HD11 | 1:118:A:LYS:HB2 | 13                  | 0.14     | 0.03                | 0.13       |
| (1,1639) | 1:115:A:LEU:HD11 | 1:118:A:LYS:HB3 | 13                  | 0.14     | 0.03                | 0.13       |
| (1,1639) | 1:115:A:LEU:HD12 | 1:118:A:LYS:HB2 | 13                  | 0.14     | 0.03                | 0.13       |
| (1,1639) | 1:115:A:LEU:HD12 | 1:118:A:LYS:HB3 | 13                  | 0.14     | 0.03                | 0.13       |
| (1,1639) | 1:115:A:LEU:HD13 | 1:118:A:LYS:HB2 | 13                  | 0.14     | 0.03                | 0.13       |
| (1,1639) | 1:115:A:LEU:HD13 | 1:118:A:LYS:HB3 | 13                  | 0.14     | 0.03                | 0.13       |
| (1,1639) | 1:115:A:LEU:HD21 | 1:118:A:LYS:HB2 | 13                  | 0.14     | 0.03                | 0.13       |
| (1,1639) | 1:115:A:LEU:HD21 | 1:118:A:LYS:HB3 | 13                  | 0.14     | 0.03                | 0.13       |
| (1,1639) | 1:115:A:LEU:HD22 | 1:118:A:LYS:HB2 | 13                  | 0.14     | 0.03                | 0.13       |
| (1,1639) | 1:115:A:LEU:HD22 | 1:118:A:LYS:HB3 | 13                  | 0.14     | 0.03                | 0.13       |
| (1,1639) | 1:115:A:LEU:HD23 | 1:118:A:LYS:HB2 | 13                  | 0.14     | 0.03                | 0.13       |
| (1,1639) | 1:115:A:LEU:HD23 | 1:118:A:LYS:HB3 | 13                  | 0.14     | 0.03                | 0.13       |
| (1,1431) | 1:147:A:HIS:H    | 1:148:A:LEU:HG  | 12                  | 0.14     | 0.02                | 0.13       |
| (1,453)  | 1:43:A:LEU:H     | 1:135:A:GLY:H   | 12                  | 0.13     | 0.02                | 0.13       |
| (1,629)  | 1:60:A:PRO:HA    | 1:62:A:GLY:H    | 11                  | 0.14     | 0.04                | 0.13       |
| (1,1145) | 1:114:A:TYR:HD1  | 1:115:A:LEU:H   | 11                  | 0.13     | 0.02                | 0.12       |
| (1,29)   | 1:6:A:PHE:H      | 1:7:A:GLU:H     | 10                  | 0.22     | 0.07                | 0.21       |
| (1,45)   | 1:9:A:SER:HA     | 1:107:A:LEU:H   | 10                  | 0.19     | 0.05                | 0.22       |
| (1,210)  | 1:22:A:ASN:H     | 1:156:A:ASP:H   | 10                  | 0.16     | 0.03                | 0.16       |
| (1,1097) | 1:108:A:SER:H    | 1:114:A:TYR:HE1 | 10                  | 0.14     | 0.02                | 0.13       |
| (1,242)  | 1:26:A:TYR:HA    | 1:46:A:LEU:H    | 10                  | 0.13     | 0.03                | 0.13       |
| (1,223)  | 1:23:A:SER:H     | 1:152:A:GLU:H   | 9                   | 0.16     | 0.04                | 0.15       |
| (1,695)  | 1:66:A:ASN:H     | 1:69:A:SER:H    | 9                   | 0.15     | 0.03                | 0.15       |
| (1,195)  | 1:21:A:ASN:H     | 1:155:A:TRP:HH2 | 9                   | 0.14     | 0.03                | 0.13       |
| (1,702)  | 1:67:A:LYS:HA    | 1:68:A:LYS:H    | 8                   | 0.1      | 0.0                 | 0.1        |
| (1,500)  | 1:47:A:ARG:H     | 1:49:A:LYS:H    | 7                   | 0.19     | 0.05                | 0.19       |
| (1,1161) | 1:115:A:LEU:HG   | 1:117:A:ASN:H   | 7                   | 0.19     | 0.06                | 0.21       |
| (1,1356) | 1:138:A:VAL:HB   | 1:138:A:VAL:H   | 7                   | 0.17     | 0.01                | 0.17       |
| (1,1294) | 1:129:A:PHE:HA   | 1:131:A:ALA:H   | 7                   | 0.15     | 0.02                | 0.15       |
| (1,285)  | 1:28:A:LEU:HG    | 1:29:A:MET:H    | 7                   | 0.15     | 0.04                | 0.15       |
| (1,545)  | 1:53:A:SER:HA    | 1:68:A:LYS:H    | 7                   | 0.13     | 0.03                | 0.12       |
| (1,286)  | 1:28:A:LEU:HG    | 1:56:A:TRP:HE1  | 7                   | 0.13     | 0.02                | 0.14       |
| (1,864)  | 1:83:A:GLY:H     | 1:139:A:HIS:HD2 | 7                   | 0.13     | 0.02                | 0.13       |
| (1,330)  | 1:31:A:ASP:HA    | 1:32:A:ASN:H    | 7                   | 0.12     | 0.01                | 0.11       |
| (1,1318) | 1:132:A:ARG:HG2  | 1:134:A:GLU:H   | 6                   | 0.17     | 0.03                | 0.18       |
| (1,1318) | 1:132:A:ARG:HG3  | 1:134:A:GLU:H   | 6                   | 0.17     | 0.03                | 0.18       |
| (1,603)  | 1:57:A:ARG:H     | 1:65:A:VAL:HB   | 6                   | 0.15     | 0.03                | 0.16       |
| (1,1479) | 1:152:A:GLU:HA   | 1:154:A:ARG:H   | 6                   | 0.13     | 0.03                | 0.12       |
| (1,130)  | 1:18:A:PHE:H     | 1:158:A:VAL:HB  | 6                   | 0.11     | 0.01                | 0.11       |
| (1,1539) | 1:161:A:VAL:HB   | 1:161:A:VAL:H   | 5                   | 0.25     | 0.06                | 0.21       |
| (1,1364) | 1:139:A:HIS:HD2  | 1:139:A:HIS:H   | 5                   | 0.18     | 0.04                | 0.19       |
| (1,1080) | 1:107:A:LEU:HA   | 1:114:A:TYR:H   | 5                   | 0.15     | 0.04                | 0.12       |

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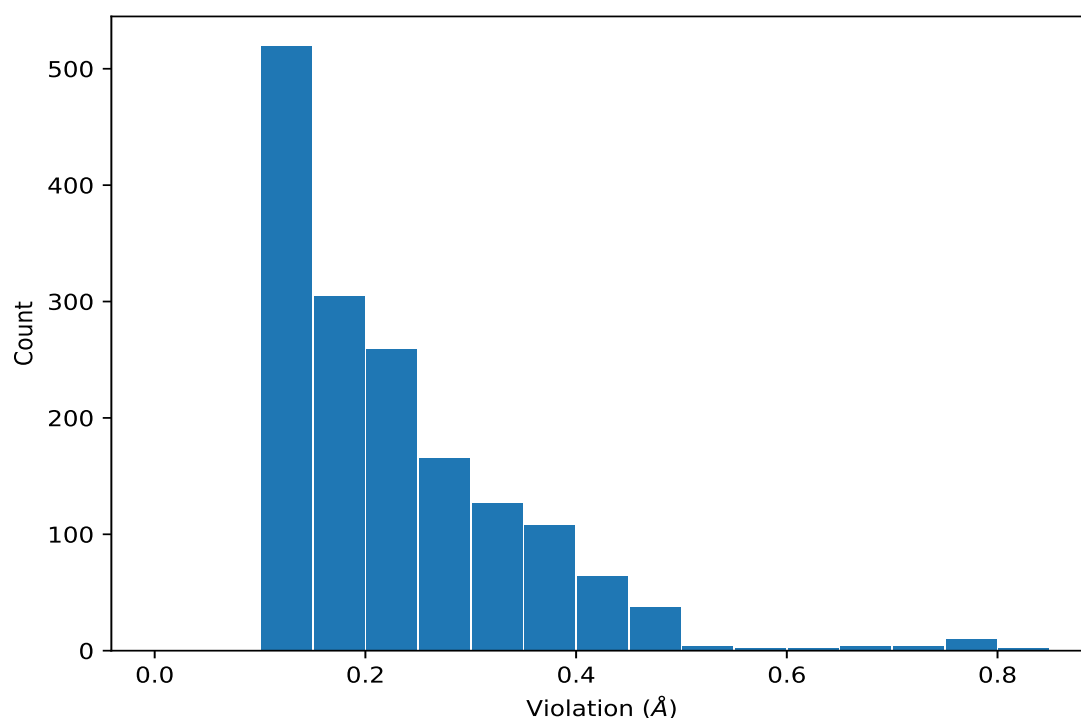
| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,374)  | 1:36:A:GLU:HA   | 1:37:A:SER:H     | 4                   | 0.4      | 0.03                | 0.42       |
| (1,1542) | 1:162:A:VAL:HB  | 1:162:A:VAL:H    | 4                   | 0.16     | 0.01                | 0.16       |
| (1,363)  | 1:34:A:SER:H    | 1:36:A:GLU:H     | 4                   | 0.16     | 0.04                | 0.15       |
| (1,999)  | 1:98:A:ASP:HA   | 1:101:A:ASN:HD22 | 4                   | 0.13     | 0.02                | 0.13       |
| (1,998)  | 1:98:A:ASP:HA   | 1:100:A:LEU:H    | 4                   | 0.13     | 0.02                | 0.13       |
| (1,754)  | 1:72:A:VAL:H    | 1:89:A:GLN:H     | 4                   | 0.12     | 0.02                | 0.12       |
| (1,1449) | 1:150:A:ARG:HA  | 1:152:A:GLU:H    | 4                   | 0.12     | 0.01                | 0.11       |
| (1,1241) | 1:123:A:LEU:HG  | 1:123:A:LEU:H    | 3                   | 0.22     | 0.09                | 0.16       |
| (1,745)  | 1:72:A:VAL:HB   | 1:73:A:MET:H     | 3                   | 0.21     | 0.04                | 0.2        |
| (1,7)    | 1:4:A:ALA:HA    | 1:6:A:PHE:H      | 3                   | 0.21     | 0.01                | 0.2        |
| (1,317)  | 1:30:A:VAL:HG11 | 1:34:A:SER:H     | 3                   | 0.21     | 0.01                | 0.21       |
| (1,317)  | 1:30:A:VAL:HG12 | 1:34:A:SER:H     | 3                   | 0.21     | 0.01                | 0.21       |
| (1,317)  | 1:30:A:VAL:HG13 | 1:34:A:SER:H     | 3                   | 0.21     | 0.01                | 0.21       |
| (1,317)  | 1:30:A:VAL:HG21 | 1:34:A:SER:H     | 3                   | 0.21     | 0.01                | 0.21       |
| (1,317)  | 1:30:A:VAL:HG22 | 1:34:A:SER:H     | 3                   | 0.21     | 0.01                | 0.21       |
| (1,317)  | 1:30:A:VAL:HG23 | 1:34:A:SER:H     | 3                   | 0.21     | 0.01                | 0.21       |
| (1,334)  | 1:31:A:ASP:H    | 1:41:A:ILE:HA    | 3                   | 0.12     | 0.01                | 0.11       |
| (1,506)  | 1:48:A:THR:HB   | 1:49:A:LYS:H     | 2                   | 0.4      | 0.02                | 0.4        |
| (1,99)   | 1:16:A:TRP:HD1  | 1:17:A:PHE:H     | 2                   | 0.27     | 0.02                | 0.27       |
| (1,968)  | 1:96:A:VAL:HB   | 1:96:A:VAL:H     | 2                   | 0.2      | 0.01                | 0.2        |
| (1,175)  | 1:20:A:LYS:H    | 1:155:A:TRP:HA   | 2                   | 0.17     | 0.0                 | 0.17       |
| (1,484)  | 1:46:A:LEU:HG   | 1:47:A:ARG:H     | 2                   | 0.14     | 0.03                | 0.14       |
| (1,1096) | 1:108:A:SER:H   | 1:112:A:HIS:H    | 2                   | 0.14     | 0.01                | 0.14       |
| (1,212)  | 1:23:A:SER:HA   | 1:152:A:GLU:H    | 2                   | 0.14     | 0.01                | 0.14       |
| (1,940)  | 1:92:A:ALA:HA   | 1:93:A:GLY:H     | 2                   | 0.13     | 0.03                | 0.13       |
| (1,612)  | 1:58:A:HIS:HD2  | 1:59:A:ASP:H     | 2                   | 0.12     | 0.02                | 0.12       |
| (1,669)  | 1:64:A:LEU:HG   | 1:65:A:VAL:H     | 2                   | 0.12     | 0.01                | 0.12       |

<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) |
|----------|----------------|----------------|----------|---------------|
| (1,1655) | 1:58:A:HIS:HE1 | 1:62:A:GLY:HA2 | 15       | 0.81          |
| (1,1655) | 1:58:A:HIS:HE1 | 1:62:A:GLY:HA3 | 15       | 0.81          |
| (1,1655) | 1:58:A:HIS:HE1 | 1:62:A:GLY:HA2 | 9        | 0.78          |
| (1,1655) | 1:58:A:HIS:HE1 | 1:62:A:GLY:HA3 | 9        | 0.78          |
| (1,1655) | 1:58:A:HIS:HE1 | 1:62:A:GLY:HA2 | 10       | 0.78          |
| (1,1655) | 1:58:A:HIS:HE1 | 1:62:A:GLY:HA3 | 10       | 0.78          |
| (1,1655) | 1:58:A:HIS:HE1 | 1:62:A:GLY:HA2 | 11       | 0.76          |
| (1,1655) | 1:58:A:HIS:HE1 | 1:62:A:GLY:HA3 | 11       | 0.76          |
| (1,1655) | 1:58:A:HIS:HE1 | 1:62:A:GLY:HA2 | 18       | 0.76          |
| (1,1655) | 1:58:A:HIS:HE1 | 1:62:A:GLY:HA3 | 18       | 0.76          |
| (1,1655) | 1:58:A:HIS:HE1 | 1:62:A:GLY:HA2 | 4        | 0.75          |
| (1,1655) | 1:58:A:HIS:HE1 | 1:62:A:GLY:HA3 | 4        | 0.75          |
| (1,1655) | 1:58:A:HIS:HE1 | 1:62:A:GLY:HA2 | 5        | 0.7           |
| (1,1655) | 1:58:A:HIS:HE1 | 1:62:A:GLY:HA3 | 5        | 0.7           |
| (1,1655) | 1:58:A:HIS:HE1 | 1:62:A:GLY:HA2 | 13       | 0.7           |
| (1,1655) | 1:58:A:HIS:HE1 | 1:62:A:GLY:HA3 | 13       | 0.7           |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1655) | 1:58:A:HIS:HE1 | 1:62:A:GLY:HA2 | 17       | 0.66          |
| (1,1655) | 1:58:A:HIS:HE1 | 1:62:A:GLY:HA3 | 17       | 0.66          |
| (1,1655) | 1:58:A:HIS:HE1 | 1:62:A:GLY:HA2 | 19       | 0.65          |
| (1,1655) | 1:58:A:HIS:HE1 | 1:62:A:GLY:HA3 | 19       | 0.65          |
| (1,1655) | 1:58:A:HIS:HE1 | 1:62:A:GLY:HA2 | 20       | 0.62          |
| (1,1655) | 1:58:A:HIS:HE1 | 1:62:A:GLY:HA3 | 20       | 0.62          |
| (1,1655) | 1:58:A:HIS:HE1 | 1:62:A:GLY:HA2 | 8        | 0.59          |
| (1,1655) | 1:58:A:HIS:HE1 | 1:62:A:GLY:HA3 | 8        | 0.59          |
| (1,1335) | 1:134:A:GLU:H  | 1:135:A:GLY:H  | 1        | 0.51          |
| (1,1335) | 1:134:A:GLU:H  | 1:135:A:GLY:H  | 4        | 0.51          |
| (1,1335) | 1:134:A:GLU:H  | 1:135:A:GLY:H  | 12       | 0.51          |
| (1,623)  | 1:59:A:ASP:H   | 1:63:A:TYR:HD1 | 6        | 0.5           |
| (1,1335) | 1:134:A:GLU:H  | 1:135:A:GLY:H  | 15       | 0.48          |
| (1,1307) | 1:131:A:ALA:H  | 1:132:A:ARG:H  | 15       | 0.48          |
| (1,1307) | 1:131:A:ALA:H  | 1:132:A:ARG:H  | 18       | 0.48          |
| (1,728)  | 1:69:A:SER:H   | 1:71:A:GLN:H   | 19       | 0.48          |
| (1,623)  | 1:59:A:ASP:H   | 1:63:A:TYR:HD1 | 17       | 0.48          |
| (1,1335) | 1:134:A:GLU:H  | 1:135:A:GLY:H  | 5        | 0.47          |
| (1,1335) | 1:134:A:GLU:H  | 1:135:A:GLY:H  | 13       | 0.47          |
| (1,1335) | 1:134:A:GLU:H  | 1:135:A:GLY:H  | 19       | 0.47          |
| (1,1008) | 1:99:A:ASP:HA  | 1:100:A:LEU:H  | 20       | 0.47          |
| (1,927)  | 1:90:A:THR:HB  | 1:91:A:GLN:H   | 11       | 0.47          |
| (1,587)  | 1:56:A:TRP:HE3 | 1:56:A:TRP:H   | 18       | 0.47          |
| (1,1357) | 1:138:A:VAL:HB | 1:139:A:HIS:H  | 6        | 0.46          |
| (1,1357) | 1:138:A:VAL:HB | 1:139:A:HIS:H  | 20       | 0.46          |
| (1,1335) | 1:134:A:GLU:H  | 1:135:A:GLY:H  | 6        | 0.46          |
| (1,1335) | 1:134:A:GLU:H  | 1:135:A:GLY:H  | 10       | 0.46          |
| (1,1335) | 1:134:A:GLU:H  | 1:135:A:GLY:H  | 11       | 0.46          |
| (1,1335) | 1:134:A:GLU:H  | 1:135:A:GLY:H  | 16       | 0.46          |
| (1,1307) | 1:131:A:ALA:H  | 1:132:A:ARG:H  | 19       | 0.46          |
| (1,1008) | 1:99:A:ASP:HA  | 1:100:A:LEU:H  | 16       | 0.46          |
| (1,601)  | 1:57:A:ARG:H   | 1:64:A:LEU:HA  | 2        | 0.46          |
| (1,601)  | 1:57:A:ARG:H   | 1:64:A:LEU:HA  | 19       | 0.46          |
| (1,587)  | 1:56:A:TRP:HE3 | 1:56:A:TRP:H   | 1        | 0.46          |
| (1,587)  | 1:56:A:TRP:HE3 | 1:56:A:TRP:H   | 3        | 0.46          |
| (1,587)  | 1:56:A:TRP:HE3 | 1:56:A:TRP:H   | 13       | 0.46          |
| (1,1335) | 1:134:A:GLU:H  | 1:135:A:GLY:H  | 9        | 0.45          |
| (1,1335) | 1:134:A:GLU:H  | 1:135:A:GLY:H  | 14       | 0.45          |
| (1,1307) | 1:131:A:ALA:H  | 1:132:A:ARG:H  | 6        | 0.45          |
| (1,851)  | 1:81:A:LYS:H   | 1:84:A:VAL:H   | 5        | 0.45          |
| (1,851)  | 1:81:A:LYS:H   | 1:84:A:VAL:H   | 6        | 0.45          |
| (1,601)  | 1:57:A:ARG:H   | 1:64:A:LEU:HA  | 20       | 0.45          |

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| Key      | Atom-1         | Atom-2        | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (1,587)  | 1:56:A:TRP:HE3 | 1:56:A:TRP:H  | 4        | 0.45          |
| (1,587)  | 1:56:A:TRP:HE3 | 1:56:A:TRP:H  | 8        | 0.45          |
| (1,587)  | 1:56:A:TRP:HE3 | 1:56:A:TRP:H  | 9        | 0.45          |
| (1,587)  | 1:56:A:TRP:HE3 | 1:56:A:TRP:H  | 11       | 0.45          |
| (1,587)  | 1:56:A:TRP:HE3 | 1:56:A:TRP:H  | 15       | 0.45          |
| (1,587)  | 1:56:A:TRP:HE3 | 1:56:A:TRP:H  | 19       | 0.45          |
| (1,587)  | 1:56:A:TRP:HE3 | 1:56:A:TRP:H  | 20       | 0.45          |
| (1,1357) | 1:138:A:VAL:HB | 1:139:A:HIS:H | 5        | 0.44          |
| (1,1357) | 1:138:A:VAL:HB | 1:139:A:HIS:H | 19       | 0.44          |
| (1,1335) | 1:134:A:GLU:H  | 1:135:A:GLY:H | 2        | 0.44          |
| (1,1335) | 1:134:A:GLU:H  | 1:135:A:GLY:H | 18       | 0.44          |
| (1,1008) | 1:99:A:ASP:HA  | 1:100:A:LEU:H | 18       | 0.44          |
| (1,601)  | 1:57:A:ARG:H   | 1:64:A:LEU:HA | 7        | 0.44          |
| (1,587)  | 1:56:A:TRP:HE3 | 1:56:A:TRP:H  | 14       | 0.44          |
| (1,587)  | 1:56:A:TRP:HE3 | 1:56:A:TRP:H  | 16       | 0.44          |
| (1,587)  | 1:56:A:TRP:HE3 | 1:56:A:TRP:H  | 17       | 0.44          |
| (1,1357) | 1:138:A:VAL:HB | 1:139:A:HIS:H | 16       | 0.43          |
| (1,1335) | 1:134:A:GLU:H  | 1:135:A:GLY:H | 3        | 0.43          |
| (1,1307) | 1:131:A:ALA:H  | 1:132:A:ARG:H | 10       | 0.43          |
| (1,1304) | 1:131:A:ALA:HA | 1:132:A:ARG:H | 3        | 0.43          |
| (1,1008) | 1:99:A:ASP:HA  | 1:100:A:LEU:H | 2        | 0.43          |
| (1,1008) | 1:99:A:ASP:HA  | 1:100:A:LEU:H | 6        | 0.43          |
| (1,1008) | 1:99:A:ASP:HA  | 1:100:A:LEU:H | 8        | 0.43          |
| (1,1008) | 1:99:A:ASP:HA  | 1:100:A:LEU:H | 12       | 0.43          |
| (1,851)  | 1:81:A:LYS:H   | 1:84:A:VAL:H  | 2        | 0.43          |
| (1,601)  | 1:57:A:ARG:H   | 1:64:A:LEU:HA | 10       | 0.43          |
| (1,587)  | 1:56:A:TRP:HE3 | 1:56:A:TRP:H  | 6        | 0.43          |
| (1,506)  | 1:48:A:THR:HB  | 1:49:A:LYS:H  | 13       | 0.43          |
| (1,374)  | 1:36:A:GLU:HA  | 1:37:A:SER:H  | 4        | 0.43          |
| (1,1335) | 1:134:A:GLU:H  | 1:135:A:GLY:H | 7        | 0.42          |
| (1,1335) | 1:134:A:GLU:H  | 1:135:A:GLY:H | 8        | 0.42          |
| (1,1335) | 1:134:A:GLU:H  | 1:135:A:GLY:H | 17       | 0.42          |
| (1,1335) | 1:134:A:GLU:H  | 1:135:A:GLY:H | 20       | 0.42          |
| (1,1008) | 1:99:A:ASP:HA  | 1:100:A:LEU:H | 1        | 0.42          |
| (1,1008) | 1:99:A:ASP:HA  | 1:100:A:LEU:H | 3        | 0.42          |
| (1,1008) | 1:99:A:ASP:HA  | 1:100:A:LEU:H | 4        | 0.42          |
| (1,1008) | 1:99:A:ASP:HA  | 1:100:A:LEU:H | 9        | 0.42          |
| (1,1008) | 1:99:A:ASP:HA  | 1:100:A:LEU:H | 14       | 0.42          |
| (1,851)  | 1:81:A:LYS:H   | 1:84:A:VAL:H  | 20       | 0.42          |
| (1,728)  | 1:69:A:SER:H   | 1:71:A:GLN:H  | 11       | 0.42          |
| (1,601)  | 1:57:A:ARG:H   | 1:64:A:LEU:HA | 15       | 0.42          |
| (1,587)  | 1:56:A:TRP:HE3 | 1:56:A:TRP:H  | 2        | 0.42          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,587)  | 1:56:A:TRP:HE3  | 1:56:A:TRP:H   | 7        | 0.42          |
| (1,587)  | 1:56:A:TRP:HE3  | 1:56:A:TRP:H   | 10       | 0.42          |
| (1,587)  | 1:56:A:TRP:HE3  | 1:56:A:TRP:H   | 12       | 0.42          |
| (1,374)  | 1:36:A:GLU:HA   | 1:37:A:SER:H   | 3        | 0.42          |
| (1,1307) | 1:131:A:ALA:H   | 1:132:A:ARG:H  | 11       | 0.41          |
| (1,1008) | 1:99:A:ASP:HA   | 1:100:A:LEU:H  | 7        | 0.41          |
| (1,1008) | 1:99:A:ASP:HA   | 1:100:A:LEU:H  | 11       | 0.41          |
| (1,1008) | 1:99:A:ASP:HA   | 1:100:A:LEU:H  | 17       | 0.41          |
| (1,851)  | 1:81:A:LYS:H    | 1:84:A:VAL:H   | 19       | 0.41          |
| (1,601)  | 1:57:A:ARG:H    | 1:64:A:LEU:HA  | 18       | 0.41          |
| (1,374)  | 1:36:A:GLU:HA   | 1:37:A:SER:H   | 15       | 0.41          |
| (1,112)  | 1:17:A:PHE:H    | 1:18:A:PHE:HE1 | 20       | 0.41          |
| (1,1357) | 1:138:A:VAL:HB  | 1:139:A:HIS:H  | 18       | 0.4           |
| (1,1307) | 1:131:A:ALA:H   | 1:132:A:ARG:H  | 9        | 0.4           |
| (1,1008) | 1:99:A:ASP:HA   | 1:100:A:LEU:H  | 5        | 0.4           |
| (1,1008) | 1:99:A:ASP:HA   | 1:100:A:LEU:H  | 10       | 0.4           |
| (1,1008) | 1:99:A:ASP:HA   | 1:100:A:LEU:H  | 13       | 0.4           |
| (1,1008) | 1:99:A:ASP:HA   | 1:100:A:LEU:H  | 15       | 0.4           |
| (1,1008) | 1:99:A:ASP:HA   | 1:100:A:LEU:H  | 19       | 0.4           |
| (1,851)  | 1:81:A:LYS:H    | 1:84:A:VAL:H   | 7        | 0.4           |
| (1,851)  | 1:81:A:LYS:H    | 1:84:A:VAL:H   | 11       | 0.4           |
| (1,728)  | 1:69:A:SER:H    | 1:71:A:GLN:H   | 3        | 0.4           |
| (1,728)  | 1:69:A:SER:H    | 1:71:A:GLN:H   | 13       | 0.4           |
| (1,728)  | 1:69:A:SER:H    | 1:71:A:GLN:H   | 16       | 0.4           |
| (1,601)  | 1:57:A:ARG:H    | 1:64:A:LEU:HA  | 12       | 0.4           |
| (1,112)  | 1:17:A:PHE:H    | 1:18:A:PHE:HE1 | 1        | 0.4           |
| (1,112)  | 1:17:A:PHE:H    | 1:18:A:PHE:HE1 | 3        | 0.4           |
| (1,112)  | 1:17:A:PHE:H    | 1:18:A:PHE:HE1 | 10       | 0.4           |
| (1,112)  | 1:17:A:PHE:H    | 1:18:A:PHE:HE1 | 16       | 0.4           |
| (1,1656) | 1:137:A:HIS:HE1 | 1:126:A:LYS:H  | 19       | 0.39          |
| (1,1402) | 1:144:A:ASP:H   | 1:145:A:LYS:H  | 12       | 0.39          |
| (1,1357) | 1:138:A:VAL:HB  | 1:139:A:HIS:H  | 7        | 0.39          |
| (1,851)  | 1:81:A:LYS:H    | 1:84:A:VAL:H   | 16       | 0.39          |
| (1,720)  | 1:68:A:LYS:H    | 1:70:A:GLY:H   | 14       | 0.39          |
| (1,587)  | 1:56:A:TRP:HE3  | 1:56:A:TRP:H   | 5        | 0.39          |
| (1,357)  | 1:34:A:SER:HA   | 1:36:A:GLU:H   | 6        | 0.39          |
| (1,112)  | 1:17:A:PHE:H    | 1:18:A:PHE:HE1 | 6        | 0.39          |
| (1,112)  | 1:17:A:PHE:H    | 1:18:A:PHE:HE1 | 8        | 0.39          |
| (1,112)  | 1:17:A:PHE:H    | 1:18:A:PHE:HE1 | 13       | 0.39          |
| (1,112)  | 1:17:A:PHE:H    | 1:18:A:PHE:HE1 | 18       | 0.39          |
| (1,1357) | 1:138:A:VAL:HB  | 1:139:A:HIS:H  | 9        | 0.38          |
| (1,1307) | 1:131:A:ALA:H   | 1:132:A:ARG:H  | 14       | 0.38          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,728)  | 1:69:A:SER:H    | 1:71:A:GLN:H   | 2        | 0.38          |
| (1,696)  | 1:66:A:ASN:H    | 1:70:A:GLY:H   | 5        | 0.38          |
| (1,696)  | 1:66:A:ASN:H    | 1:70:A:GLY:H   | 9        | 0.38          |
| (1,601)  | 1:57:A:ARG:H    | 1:64:A:LEU:HA  | 9        | 0.38          |
| (1,601)  | 1:57:A:ARG:H    | 1:64:A:LEU:HA  | 14       | 0.38          |
| (1,506)  | 1:48:A:THR:HB   | 1:49:A:LYS:H   | 20       | 0.38          |
| (1,253)  | 1:26:A:TYR:HE1  | 1:45:A:THR:H   | 6        | 0.38          |
| (1,253)  | 1:26:A:TYR:HE2  | 1:45:A:THR:H   | 6        | 0.38          |
| (1,253)  | 1:26:A:TYR:HE1  | 1:45:A:THR:H   | 11       | 0.38          |
| (1,253)  | 1:26:A:TYR:HE2  | 1:45:A:THR:H   | 11       | 0.38          |
| (1,112)  | 1:17:A:PHE:H    | 1:18:A:PHE:HE1 | 5        | 0.38          |
| (1,112)  | 1:17:A:PHE:H    | 1:18:A:PHE:HE1 | 7        | 0.38          |
| (1,112)  | 1:17:A:PHE:H    | 1:18:A:PHE:HE1 | 12       | 0.38          |
| (1,1357) | 1:138:A:VAL:HB  | 1:139:A:HIS:H  | 11       | 0.37          |
| (1,1357) | 1:138:A:VAL:HB  | 1:139:A:HIS:H  | 12       | 0.37          |
| (1,1357) | 1:138:A:VAL:HB  | 1:139:A:HIS:H  | 15       | 0.37          |
| (1,1307) | 1:131:A:ALA:H   | 1:132:A:ARG:H  | 20       | 0.37          |
| (1,1162) | 1:115:A:LEU:HG  | 1:118:A:LYS:H  | 11       | 0.37          |
| (1,812)  | 1:77:A:LYS:HA   | 1:79:A:THR:H   | 2        | 0.37          |
| (1,728)  | 1:69:A:SER:H    | 1:71:A:GLN:H   | 7        | 0.37          |
| (1,728)  | 1:69:A:SER:H    | 1:71:A:GLN:H   | 10       | 0.37          |
| (1,728)  | 1:69:A:SER:H    | 1:71:A:GLN:H   | 12       | 0.37          |
| (1,720)  | 1:68:A:LYS:H    | 1:70:A:GLY:H   | 4        | 0.37          |
| (1,696)  | 1:66:A:ASN:H    | 1:70:A:GLY:H   | 4        | 0.37          |
| (1,696)  | 1:66:A:ASN:H    | 1:70:A:GLY:H   | 17       | 0.37          |
| (1,601)  | 1:57:A:ARG:H    | 1:64:A:LEU:HA  | 3        | 0.37          |
| (1,601)  | 1:57:A:ARG:H    | 1:64:A:LEU:HA  | 4        | 0.37          |
| (1,601)  | 1:57:A:ARG:H    | 1:64:A:LEU:HA  | 11       | 0.37          |
| (1,253)  | 1:26:A:TYR:HE1  | 1:45:A:THR:H   | 18       | 0.37          |
| (1,253)  | 1:26:A:TYR:HE2  | 1:45:A:THR:H   | 18       | 0.37          |
| (1,112)  | 1:17:A:PHE:H    | 1:18:A:PHE:HE1 | 4        | 0.37          |
| (1,112)  | 1:17:A:PHE:H    | 1:18:A:PHE:HE1 | 9        | 0.37          |
| (1,112)  | 1:17:A:PHE:H    | 1:18:A:PHE:HE1 | 15       | 0.37          |
| (1,112)  | 1:17:A:PHE:H    | 1:18:A:PHE:HE1 | 19       | 0.37          |
| (1,1656) | 1:137:A:HIS:HE1 | 1:126:A:LYS:H  | 5        | 0.36          |
| (1,1656) | 1:137:A:HIS:HE1 | 1:126:A:LYS:H  | 9        | 0.36          |
| (1,1656) | 1:137:A:HIS:HE1 | 1:126:A:LYS:H  | 10       | 0.36          |
| (1,1357) | 1:138:A:VAL:HB  | 1:139:A:HIS:H  | 13       | 0.36          |
| (1,1310) | 1:132:A:ARG:HA  | 1:134:A:GLU:H  | 7        | 0.36          |
| (1,1162) | 1:115:A:LEU:HG  | 1:118:A:LYS:H  | 4        | 0.36          |
| (1,1162) | 1:115:A:LEU:HG  | 1:118:A:LYS:H  | 6        | 0.36          |
| (1,1162) | 1:115:A:LEU:HG  | 1:118:A:LYS:H  | 12       | 0.36          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1162) | 1:115:A:LEU:HG  | 1:118:A:LYS:H  | 17       | 0.36          |
| (1,1162) | 1:115:A:LEU:HG  | 1:118:A:LYS:H  | 20       | 0.36          |
| (1,851)  | 1:81:A:LYS:H    | 1:84:A:VAL:H   | 13       | 0.36          |
| (1,851)  | 1:81:A:LYS:H    | 1:84:A:VAL:H   | 15       | 0.36          |
| (1,812)  | 1:77:A:LYS:HA   | 1:79:A:THR:H   | 3        | 0.36          |
| (1,812)  | 1:77:A:LYS:HA   | 1:79:A:THR:H   | 7        | 0.36          |
| (1,812)  | 1:77:A:LYS:HA   | 1:79:A:THR:H   | 11       | 0.36          |
| (1,812)  | 1:77:A:LYS:HA   | 1:79:A:THR:H   | 17       | 0.36          |
| (1,812)  | 1:77:A:LYS:HA   | 1:79:A:THR:H   | 19       | 0.36          |
| (1,812)  | 1:77:A:LYS:HA   | 1:79:A:THR:H   | 20       | 0.36          |
| (1,728)  | 1:69:A:SER:H    | 1:71:A:GLN:H   | 1        | 0.36          |
| (1,720)  | 1:68:A:LYS:H    | 1:70:A:GLY:H   | 5        | 0.36          |
| (1,720)  | 1:68:A:LYS:H    | 1:70:A:GLY:H   | 17       | 0.36          |
| (1,601)  | 1:57:A:ARG:H    | 1:64:A:LEU:HA  | 1        | 0.36          |
| (1,601)  | 1:57:A:ARG:H    | 1:64:A:LEU:HA  | 16       | 0.36          |
| (1,549)  | 1:53:A:SER:H    | 1:55:A:LEU:H   | 8        | 0.36          |
| (1,374)  | 1:36:A:GLU:HA   | 1:37:A:SER:H   | 5        | 0.36          |
| (1,112)  | 1:17:A:PHE:H    | 1:18:A:PHE:HE1 | 14       | 0.36          |
| (1,1656) | 1:137:A:HIS:HE1 | 1:126:A:LYS:H  | 14       | 0.35          |
| (1,1402) | 1:144:A:ASP:H   | 1:145:A:LYS:H  | 4        | 0.35          |
| (1,1357) | 1:138:A:VAL:HB  | 1:139:A:HIS:H  | 3        | 0.35          |
| (1,1357) | 1:138:A:VAL:HB  | 1:139:A:HIS:H  | 10       | 0.35          |
| (1,1357) | 1:138:A:VAL:HB  | 1:139:A:HIS:H  | 17       | 0.35          |
| (1,1241) | 1:123:A:LEU:HG  | 1:123:A:LEU:H  | 2        | 0.35          |
| (1,1162) | 1:115:A:LEU:HG  | 1:118:A:LYS:H  | 13       | 0.35          |
| (1,1162) | 1:115:A:LEU:HG  | 1:118:A:LYS:H  | 14       | 0.35          |
| (1,851)  | 1:81:A:LYS:H    | 1:84:A:VAL:H   | 4        | 0.35          |
| (1,812)  | 1:77:A:LYS:HA   | 1:79:A:THR:H   | 1        | 0.35          |
| (1,812)  | 1:77:A:LYS:HA   | 1:79:A:THR:H   | 5        | 0.35          |
| (1,812)  | 1:77:A:LYS:HA   | 1:79:A:THR:H   | 8        | 0.35          |
| (1,812)  | 1:77:A:LYS:HA   | 1:79:A:THR:H   | 12       | 0.35          |
| (1,812)  | 1:77:A:LYS:HA   | 1:79:A:THR:H   | 13       | 0.35          |
| (1,812)  | 1:77:A:LYS:HA   | 1:79:A:THR:H   | 14       | 0.35          |
| (1,812)  | 1:77:A:LYS:HA   | 1:79:A:THR:H   | 16       | 0.35          |
| (1,728)  | 1:69:A:SER:H    | 1:71:A:GLN:H   | 8        | 0.35          |
| (1,728)  | 1:69:A:SER:H    | 1:71:A:GLN:H   | 15       | 0.35          |
| (1,728)  | 1:69:A:SER:H    | 1:71:A:GLN:H   | 18       | 0.35          |
| (1,720)  | 1:68:A:LYS:H    | 1:70:A:GLY:H   | 9        | 0.35          |
| (1,601)  | 1:57:A:ARG:H    | 1:64:A:LEU:HA  | 8        | 0.35          |
| (1,601)  | 1:57:A:ARG:H    | 1:64:A:LEU:HA  | 13       | 0.35          |
| (1,549)  | 1:53:A:SER:H    | 1:55:A:LEU:H   | 1        | 0.35          |
| (1,549)  | 1:53:A:SER:H    | 1:55:A:LEU:H   | 4        | 0.35          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,549)  | 1:53:A:SER:H    | 1:55:A:LEU:H   | 6        | 0.35          |
| (1,549)  | 1:53:A:SER:H    | 1:55:A:LEU:H   | 14       | 0.35          |
| (1,468)  | 1:45:A:THR:HB   | 1:46:A:LEU:H   | 5        | 0.35          |
| (1,253)  | 1:26:A:TYR:HE1  | 1:45:A:THR:H   | 15       | 0.35          |
| (1,253)  | 1:26:A:TYR:HE2  | 1:45:A:THR:H   | 15       | 0.35          |
| (1,253)  | 1:26:A:TYR:HE1  | 1:45:A:THR:H   | 19       | 0.35          |
| (1,253)  | 1:26:A:TYR:HE2  | 1:45:A:THR:H   | 19       | 0.35          |
| (1,116)  | 1:17:A:PHE:H    | 1:56:A:TRP:HD1 | 5        | 0.35          |
| (1,112)  | 1:17:A:PHE:H    | 1:18:A:PHE:HE1 | 2        | 0.35          |
| (1,112)  | 1:17:A:PHE:H    | 1:18:A:PHE:HE1 | 11       | 0.35          |
| (1,112)  | 1:17:A:PHE:H    | 1:18:A:PHE:HE1 | 17       | 0.35          |
| (1,1656) | 1:137:A:HIS:HE1 | 1:126:A:LYS:H  | 11       | 0.34          |
| (1,1656) | 1:137:A:HIS:HE1 | 1:126:A:LYS:H  | 13       | 0.34          |
| (1,1656) | 1:137:A:HIS:HE1 | 1:126:A:LYS:H  | 20       | 0.34          |
| (1,1357) | 1:138:A:VAL:HB  | 1:139:A:HIS:H  | 1        | 0.34          |
| (1,1307) | 1:131:A:ALA:H   | 1:132:A:ARG:H  | 7        | 0.34          |
| (1,1162) | 1:115:A:LEU:HG  | 1:118:A:LYS:H  | 3        | 0.34          |
| (1,1162) | 1:115:A:LEU:HG  | 1:118:A:LYS:H  | 8        | 0.34          |
| (1,1162) | 1:115:A:LEU:HG  | 1:118:A:LYS:H  | 18       | 0.34          |
| (1,851)  | 1:81:A:LYS:H    | 1:84:A:VAL:H   | 1        | 0.34          |
| (1,851)  | 1:81:A:LYS:H    | 1:84:A:VAL:H   | 3        | 0.34          |
| (1,812)  | 1:77:A:LYS:HA   | 1:79:A:THR:H   | 4        | 0.34          |
| (1,812)  | 1:77:A:LYS:HA   | 1:79:A:THR:H   | 6        | 0.34          |
| (1,812)  | 1:77:A:LYS:HA   | 1:79:A:THR:H   | 9        | 0.34          |
| (1,812)  | 1:77:A:LYS:HA   | 1:79:A:THR:H   | 10       | 0.34          |
| (1,812)  | 1:77:A:LYS:HA   | 1:79:A:THR:H   | 15       | 0.34          |
| (1,812)  | 1:77:A:LYS:HA   | 1:79:A:THR:H   | 18       | 0.34          |
| (1,720)  | 1:68:A:LYS:H    | 1:70:A:GLY:H   | 6        | 0.34          |
| (1,720)  | 1:68:A:LYS:H    | 1:70:A:GLY:H   | 10       | 0.34          |
| (1,720)  | 1:68:A:LYS:H    | 1:70:A:GLY:H   | 19       | 0.34          |
| (1,549)  | 1:53:A:SER:H    | 1:55:A:LEU:H   | 3        | 0.34          |
| (1,549)  | 1:53:A:SER:H    | 1:55:A:LEU:H   | 10       | 0.34          |
| (1,549)  | 1:53:A:SER:H    | 1:55:A:LEU:H   | 13       | 0.34          |
| (1,549)  | 1:53:A:SER:H    | 1:55:A:LEU:H   | 16       | 0.34          |
| (1,549)  | 1:53:A:SER:H    | 1:55:A:LEU:H   | 17       | 0.34          |
| (1,468)  | 1:45:A:THR:HB   | 1:46:A:LEU:H   | 1        | 0.34          |
| (1,468)  | 1:45:A:THR:HB   | 1:46:A:LEU:H   | 2        | 0.34          |
| (1,468)  | 1:45:A:THR:HB   | 1:46:A:LEU:H   | 16       | 0.34          |
| (1,357)  | 1:34:A:SER:HA   | 1:36:A:GLU:H   | 16       | 0.34          |
| (1,225)  | 1:23:A:SER:H    | 1:25:A:GLY:H   | 19       | 0.34          |
| (1,116)  | 1:17:A:PHE:H    | 1:56:A:TRP:HD1 | 2        | 0.34          |
| (1,116)  | 1:17:A:PHE:H    | 1:56:A:TRP:HD1 | 15       | 0.34          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1656) | 1:137:A:HIS:HE1 | 1:126:A:LYS:H  | 12       | 0.33          |
| (1,1357) | 1:138:A:VAL:HB  | 1:139:A:HIS:H  | 4        | 0.33          |
| (1,1357) | 1:138:A:VAL:HB  | 1:139:A:HIS:H  | 8        | 0.33          |
| (1,1357) | 1:138:A:VAL:HB  | 1:139:A:HIS:H  | 14       | 0.33          |
| (1,1310) | 1:132:A:ARG:HA  | 1:134:A:GLU:H  | 10       | 0.33          |
| (1,1307) | 1:131:A:ALA:H   | 1:132:A:ARG:H  | 8        | 0.33          |
| (1,1162) | 1:115:A:LEU:HG  | 1:118:A:LYS:H  | 16       | 0.33          |
| (1,1162) | 1:115:A:LEU:HG  | 1:118:A:LYS:H  | 19       | 0.33          |
| (1,960)  | 1:95:A:ASN:HA   | 1:96:A:VAL:H   | 18       | 0.33          |
| (1,851)  | 1:81:A:LYS:H    | 1:84:A:VAL:H   | 12       | 0.33          |
| (1,851)  | 1:81:A:LYS:H    | 1:84:A:VAL:H   | 14       | 0.33          |
| (1,720)  | 1:68:A:LYS:H    | 1:70:A:GLY:H   | 2        | 0.33          |
| (1,720)  | 1:68:A:LYS:H    | 1:70:A:GLY:H   | 8        | 0.33          |
| (1,720)  | 1:68:A:LYS:H    | 1:70:A:GLY:H   | 12       | 0.33          |
| (1,720)  | 1:68:A:LYS:H    | 1:70:A:GLY:H   | 20       | 0.33          |
| (1,696)  | 1:66:A:ASN:H    | 1:70:A:GLY:H   | 6        | 0.33          |
| (1,549)  | 1:53:A:SER:H    | 1:55:A:LEU:H   | 9        | 0.33          |
| (1,549)  | 1:53:A:SER:H    | 1:55:A:LEU:H   | 20       | 0.33          |
| (1,468)  | 1:45:A:THR:HB   | 1:46:A:LEU:H   | 7        | 0.33          |
| (1,468)  | 1:45:A:THR:HB   | 1:46:A:LEU:H   | 10       | 0.33          |
| (1,468)  | 1:45:A:THR:HB   | 1:46:A:LEU:H   | 18       | 0.33          |
| (1,357)  | 1:34:A:SER:HA   | 1:36:A:GLU:H   | 13       | 0.33          |
| (1,357)  | 1:34:A:SER:HA   | 1:36:A:GLU:H   | 18       | 0.33          |
| (1,116)  | 1:17:A:PHE:H    | 1:56:A:TRP:HD1 | 19       | 0.33          |
| (1,1656) | 1:137:A:HIS:HE1 | 1:126:A:LYS:H  | 1        | 0.32          |
| (1,1656) | 1:137:A:HIS:HE1 | 1:126:A:LYS:H  | 16       | 0.32          |
| (1,1656) | 1:137:A:HIS:HE1 | 1:126:A:LYS:H  | 18       | 0.32          |
| (1,1539) | 1:161:A:VAL:HB  | 1:161:A:VAL:H  | 3        | 0.32          |
| (1,1539) | 1:161:A:VAL:HB  | 1:161:A:VAL:H  | 13       | 0.32          |
| (1,1310) | 1:132:A:ARG:HA  | 1:134:A:GLU:H  | 9        | 0.32          |
| (1,1307) | 1:131:A:ALA:H   | 1:132:A:ARG:H  | 2        | 0.32          |
| (1,1162) | 1:115:A:LEU:HG  | 1:118:A:LYS:H  | 1        | 0.32          |
| (1,1162) | 1:115:A:LEU:HG  | 1:118:A:LYS:H  | 2        | 0.32          |
| (1,960)  | 1:95:A:ASN:HA   | 1:96:A:VAL:H   | 1        | 0.32          |
| (1,851)  | 1:81:A:LYS:H    | 1:84:A:VAL:H   | 8        | 0.32          |
| (1,851)  | 1:81:A:LYS:H    | 1:84:A:VAL:H   | 9        | 0.32          |
| (1,720)  | 1:68:A:LYS:H    | 1:70:A:GLY:H   | 11       | 0.32          |
| (1,720)  | 1:68:A:LYS:H    | 1:70:A:GLY:H   | 18       | 0.32          |
| (1,696)  | 1:66:A:ASN:H    | 1:70:A:GLY:H   | 14       | 0.32          |
| (1,601)  | 1:57:A:ARG:H    | 1:64:A:LEU:HA  | 5        | 0.32          |
| (1,549)  | 1:53:A:SER:H    | 1:55:A:LEU:H   | 11       | 0.32          |
| (1,549)  | 1:53:A:SER:H    | 1:55:A:LEU:H   | 18       | 0.32          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,488)  | 1:47:A:ARG:HA   | 1:49:A:LYS:H   | 8        | 0.32          |
| (1,357)  | 1:34:A:SER:HA   | 1:36:A:GLU:H   | 17       | 0.32          |
| (1,284)  | 1:28:A:LEU:HG   | 1:28:A:LEU:H   | 13       | 0.32          |
| (1,225)  | 1:23:A:SER:H    | 1:25:A:GLY:H   | 14       | 0.32          |
| (1,225)  | 1:23:A:SER:H    | 1:25:A:GLY:H   | 16       | 0.32          |
| (1,116)  | 1:17:A:PHE:H    | 1:56:A:TRP:HD1 | 4        | 0.32          |
| (1,116)  | 1:17:A:PHE:H    | 1:56:A:TRP:HD1 | 18       | 0.32          |
| (1,29)   | 1:6:A:PHE:H     | 1:7:A:GLU:H    | 5        | 0.32          |
| (1,29)   | 1:6:A:PHE:H     | 1:7:A:GLU:H    | 14       | 0.32          |
| (1,1357) | 1:138:A:VAL:HB  | 1:139:A:HIS:H  | 2        | 0.31          |
| (1,1310) | 1:132:A:ARG:HA  | 1:134:A:GLU:H  | 2        | 0.31          |
| (1,1310) | 1:132:A:ARG:HA  | 1:134:A:GLU:H  | 11       | 0.31          |
| (1,1162) | 1:115:A:LEU:HG  | 1:118:A:LYS:H  | 15       | 0.31          |
| (1,1073) | 1:106:A:GLY:H   | 1:114:A:TYR:H  | 3        | 0.31          |
| (1,1016) | 1:99:A:ASP:H    | 1:101:A:ASN:H  | 15       | 0.31          |
| (1,1016) | 1:99:A:ASP:H    | 1:101:A:ASN:H  | 19       | 0.31          |
| (1,851)  | 1:81:A:LYS:H    | 1:84:A:VAL:H   | 10       | 0.31          |
| (1,851)  | 1:81:A:LYS:H    | 1:84:A:VAL:H   | 18       | 0.31          |
| (1,720)  | 1:68:A:LYS:H    | 1:70:A:GLY:H   | 1        | 0.31          |
| (1,720)  | 1:68:A:LYS:H    | 1:70:A:GLY:H   | 16       | 0.31          |
| (1,696)  | 1:66:A:ASN:H    | 1:70:A:GLY:H   | 15       | 0.31          |
| (1,601)  | 1:57:A:ARG:H    | 1:64:A:LEU:HA  | 6        | 0.31          |
| (1,549)  | 1:53:A:SER:H    | 1:55:A:LEU:H   | 2        | 0.31          |
| (1,549)  | 1:53:A:SER:H    | 1:55:A:LEU:H   | 5        | 0.31          |
| (1,549)  | 1:53:A:SER:H    | 1:55:A:LEU:H   | 12       | 0.31          |
| (1,549)  | 1:53:A:SER:H    | 1:55:A:LEU:H   | 19       | 0.31          |
| (1,488)  | 1:47:A:ARG:HA   | 1:49:A:LYS:H   | 9        | 0.31          |
| (1,468)  | 1:45:A:THR:HB   | 1:46:A:LEU:H   | 14       | 0.31          |
| (1,357)  | 1:34:A:SER:HA   | 1:36:A:GLU:H   | 12       | 0.31          |
| (1,357)  | 1:34:A:SER:HA   | 1:36:A:GLU:H   | 14       | 0.31          |
| (1,225)  | 1:23:A:SER:H    | 1:25:A:GLY:H   | 10       | 0.31          |
| (1,1656) | 1:137:A:HIS:HE1 | 1:126:A:LYS:H  | 2        | 0.3           |
| (1,1461) | 1:150:A:ARG:H   | 1:152:A:GLU:H  | 13       | 0.3           |
| (1,1402) | 1:144:A:ASP:H   | 1:145:A:LYS:H  | 18       | 0.3           |
| (1,1310) | 1:132:A:ARG:HA  | 1:134:A:GLU:H  | 6        | 0.3           |
| (1,1310) | 1:132:A:ARG:HA  | 1:134:A:GLU:H  | 19       | 0.3           |
| (1,1162) | 1:115:A:LEU:HG  | 1:118:A:LYS:H  | 10       | 0.3           |
| (1,1073) | 1:106:A:GLY:H   | 1:114:A:TYR:H  | 12       | 0.3           |
| (1,1018) | 1:100:A:LEU:HA  | 1:101:A:ASN:H  | 5        | 0.3           |
| (1,1018) | 1:100:A:LEU:HA  | 1:101:A:ASN:H  | 9        | 0.3           |
| (1,1018) | 1:100:A:LEU:HA  | 1:101:A:ASN:H  | 15       | 0.3           |
| (1,1018) | 1:100:A:LEU:HA  | 1:101:A:ASN:H  | 17       | 0.3           |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,851)  | 1:81:A:LYS:H   | 1:84:A:VAL:H   | 17       | 0.3           |
| (1,696)  | 1:66:A:ASN:H   | 1:70:A:GLY:H   | 20       | 0.3           |
| (1,549)  | 1:53:A:SER:H   | 1:55:A:LEU:H   | 7        | 0.3           |
| (1,488)  | 1:47:A:ARG:HA  | 1:49:A:LYS:H   | 3        | 0.3           |
| (1,488)  | 1:47:A:ARG:HA  | 1:49:A:LYS:H   | 15       | 0.3           |
| (1,357)  | 1:34:A:SER:HA  | 1:36:A:GLU:H   | 2        | 0.3           |
| (1,284)  | 1:28:A:LEU:HG  | 1:28:A:LEU:H   | 20       | 0.3           |
| (1,253)  | 1:26:A:TYR:HE1 | 1:45:A:THR:H   | 9        | 0.3           |
| (1,253)  | 1:26:A:TYR:HE2 | 1:45:A:THR:H   | 9        | 0.3           |
| (1,225)  | 1:23:A:SER:H   | 1:25:A:GLY:H   | 12       | 0.3           |
| (1,116)  | 1:17:A:PHE:H   | 1:56:A:TRP:HD1 | 7        | 0.3           |
| (1,116)  | 1:17:A:PHE:H   | 1:56:A:TRP:HD1 | 14       | 0.3           |
| (1,1655) | 1:58:A:HIS:HE1 | 1:62:A:GLY:HA2 | 6        | 0.29          |
| (1,1655) | 1:58:A:HIS:HE1 | 1:62:A:GLY:HA3 | 6        | 0.29          |
| (1,1525) | 1:158:A:VAL:HB | 1:159:A:LEU:H  | 3        | 0.29          |
| (1,1525) | 1:158:A:VAL:HB | 1:159:A:LEU:H  | 20       | 0.29          |
| (1,1461) | 1:150:A:ARG:H  | 1:152:A:GLU:H  | 3        | 0.29          |
| (1,1402) | 1:144:A:ASP:H  | 1:145:A:LYS:H  | 7        | 0.29          |
| (1,1402) | 1:144:A:ASP:H  | 1:145:A:LYS:H  | 14       | 0.29          |
| (1,1402) | 1:144:A:ASP:H  | 1:145:A:LYS:H  | 17       | 0.29          |
| (1,1310) | 1:132:A:ARG:HA | 1:134:A:GLU:H  | 8        | 0.29          |
| (1,1307) | 1:131:A:ALA:H  | 1:132:A:ARG:H  | 17       | 0.29          |
| (1,1162) | 1:115:A:LEU:HG | 1:118:A:LYS:H  | 7        | 0.29          |
| (1,1073) | 1:106:A:GLY:H  | 1:114:A:TYR:H  | 6        | 0.29          |
| (1,1073) | 1:106:A:GLY:H  | 1:114:A:TYR:H  | 13       | 0.29          |
| (1,1073) | 1:106:A:GLY:H  | 1:114:A:TYR:H  | 14       | 0.29          |
| (1,1018) | 1:100:A:LEU:HA | 1:101:A:ASN:H  | 7        | 0.29          |
| (1,1018) | 1:100:A:LEU:HA | 1:101:A:ASN:H  | 10       | 0.29          |
| (1,1018) | 1:100:A:LEU:HA | 1:101:A:ASN:H  | 13       | 0.29          |
| (1,1018) | 1:100:A:LEU:HA | 1:101:A:ASN:H  | 19       | 0.29          |
| (1,1016) | 1:99:A:ASP:H   | 1:101:A:ASN:H  | 5        | 0.29          |
| (1,1016) | 1:99:A:ASP:H   | 1:101:A:ASN:H  | 10       | 0.29          |
| (1,1016) | 1:99:A:ASP:H   | 1:101:A:ASN:H  | 13       | 0.29          |
| (1,720)  | 1:68:A:LYS:H   | 1:70:A:GLY:H   | 7        | 0.29          |
| (1,696)  | 1:66:A:ASN:H   | 1:70:A:GLY:H   | 1        | 0.29          |
| (1,549)  | 1:53:A:SER:H   | 1:55:A:LEU:H   | 15       | 0.29          |
| (1,357)  | 1:34:A:SER:HA  | 1:36:A:GLU:H   | 7        | 0.29          |
| (1,357)  | 1:34:A:SER:HA  | 1:36:A:GLU:H   | 8        | 0.29          |
| (1,357)  | 1:34:A:SER:HA  | 1:36:A:GLU:H   | 20       | 0.29          |
| (1,284)  | 1:28:A:LEU:HG  | 1:28:A:LEU:H   | 16       | 0.29          |
| (1,225)  | 1:23:A:SER:H   | 1:25:A:GLY:H   | 9        | 0.29          |
| (1,116)  | 1:17:A:PHE:H   | 1:56:A:TRP:HD1 | 11       | 0.29          |

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| Key      | Atom-1          | Atom-2        | Model ID | Violation (Å) |
|----------|-----------------|---------------|----------|---------------|
| (1,99)   | 1:16:A:TRP:HD1  | 1:17:A:PHE:H  | 20       | 0.29          |
| (1,1656) | 1:137:A:HIS:HE1 | 1:126:A:LYS:H | 6        | 0.28          |
| (1,1525) | 1:158:A:VAL:HB  | 1:159:A:LEU:H | 8        | 0.28          |
| (1,1525) | 1:158:A:VAL:HB  | 1:159:A:LEU:H | 9        | 0.28          |
| (1,1485) | 1:152:A:GLU:H   | 1:154:A:ARG:H | 2        | 0.28          |
| (1,1442) | 1:149:A:ASP:HA  | 1:150:A:ARG:H | 9        | 0.28          |
| (1,1402) | 1:144:A:ASP:H   | 1:145:A:LYS:H | 3        | 0.28          |
| (1,1310) | 1:132:A:ARG:HA  | 1:134:A:GLU:H | 15       | 0.28          |
| (1,1310) | 1:132:A:ARG:HA  | 1:134:A:GLU:H | 18       | 0.28          |
| (1,1163) | 1:115:A:LEU:HG  | 1:120:A:SER:H | 4        | 0.28          |
| (1,1163) | 1:115:A:LEU:HG  | 1:120:A:SER:H | 8        | 0.28          |
| (1,1162) | 1:115:A:LEU:HG  | 1:118:A:LYS:H | 5        | 0.28          |
| (1,1073) | 1:106:A:GLY:H   | 1:114:A:TYR:H | 7        | 0.28          |
| (1,1073) | 1:106:A:GLY:H   | 1:114:A:TYR:H | 8        | 0.28          |
| (1,1016) | 1:99:A:ASP:H    | 1:101:A:ASN:H | 7        | 0.28          |
| (1,696)  | 1:66:A:ASN:H    | 1:70:A:GLY:H  | 8        | 0.28          |
| (1,696)  | 1:66:A:ASN:H    | 1:70:A:GLY:H  | 18       | 0.28          |
| (1,488)  | 1:47:A:ARG:HA   | 1:49:A:LYS:H  | 1        | 0.28          |
| (1,284)  | 1:28:A:LEU:HG   | 1:28:A:LEU:H  | 6        | 0.28          |
| (1,253)  | 1:26:A:TYR:HE1  | 1:45:A:THR:H  | 3        | 0.28          |
| (1,253)  | 1:26:A:TYR:HE2  | 1:45:A:THR:H  | 3        | 0.28          |
| (1,253)  | 1:26:A:TYR:HE1  | 1:45:A:THR:H  | 8        | 0.28          |
| (1,253)  | 1:26:A:TYR:HE2  | 1:45:A:THR:H  | 8        | 0.28          |
| (1,1656) | 1:137:A:HIS:HE1 | 1:126:A:LYS:H | 4        | 0.27          |
| (1,1525) | 1:158:A:VAL:HB  | 1:159:A:LEU:H | 10       | 0.27          |
| (1,1525) | 1:158:A:VAL:HB  | 1:159:A:LEU:H | 11       | 0.27          |
| (1,1525) | 1:158:A:VAL:HB  | 1:159:A:LEU:H | 15       | 0.27          |
| (1,1525) | 1:158:A:VAL:HB  | 1:159:A:LEU:H | 18       | 0.27          |
| (1,1525) | 1:158:A:VAL:HB  | 1:159:A:LEU:H | 19       | 0.27          |
| (1,1485) | 1:152:A:GLU:H   | 1:154:A:ARG:H | 1        | 0.27          |
| (1,1485) | 1:152:A:GLU:H   | 1:154:A:ARG:H | 16       | 0.27          |
| (1,1461) | 1:150:A:ARG:H   | 1:152:A:GLU:H | 14       | 0.27          |
| (1,1461) | 1:150:A:ARG:H   | 1:152:A:GLU:H | 15       | 0.27          |
| (1,1461) | 1:150:A:ARG:H   | 1:152:A:GLU:H | 18       | 0.27          |
| (1,1461) | 1:150:A:ARG:H   | 1:152:A:GLU:H | 20       | 0.27          |
| (1,1442) | 1:149:A:ASP:HA  | 1:150:A:ARG:H | 2        | 0.27          |
| (1,1402) | 1:144:A:ASP:H   | 1:145:A:LYS:H | 9        | 0.27          |
| (1,1310) | 1:132:A:ARG:HA  | 1:134:A:GLU:H | 17       | 0.27          |
| (1,1163) | 1:115:A:LEU:HG  | 1:120:A:SER:H | 3        | 0.27          |
| (1,1163) | 1:115:A:LEU:HG  | 1:120:A:SER:H | 13       | 0.27          |
| (1,1163) | 1:115:A:LEU:HG  | 1:120:A:SER:H | 14       | 0.27          |
| (1,1162) | 1:115:A:LEU:HG  | 1:118:A:LYS:H | 9        | 0.27          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1073) | 1:106:A:GLY:H   | 1:114:A:TYR:H  | 5        | 0.27          |
| (1,1073) | 1:106:A:GLY:H   | 1:114:A:TYR:H  | 17       | 0.27          |
| (1,1073) | 1:106:A:GLY:H   | 1:114:A:TYR:H  | 18       | 0.27          |
| (1,1073) | 1:106:A:GLY:H   | 1:114:A:TYR:H  | 20       | 0.27          |
| (1,1018) | 1:100:A:LEU:HA  | 1:101:A:ASN:H  | 4        | 0.27          |
| (1,1018) | 1:100:A:LEU:HA  | 1:101:A:ASN:H  | 12       | 0.27          |
| (1,745)  | 1:72:A:VAL:HB   | 1:73:A:MET:H   | 1        | 0.27          |
| (1,720)  | 1:68:A:LYS:H    | 1:70:A:GLY:H   | 3        | 0.27          |
| (1,720)  | 1:68:A:LYS:H    | 1:70:A:GLY:H   | 13       | 0.27          |
| (1,720)  | 1:68:A:LYS:H    | 1:70:A:GLY:H   | 15       | 0.27          |
| (1,623)  | 1:59:A:ASP:H    | 1:63:A:TYR:HD1 | 3        | 0.27          |
| (1,623)  | 1:59:A:ASP:H    | 1:63:A:TYR:HD1 | 9        | 0.27          |
| (1,488)  | 1:47:A:ARG:HA   | 1:49:A:LYS:H   | 7        | 0.27          |
| (1,284)  | 1:28:A:LEU:HG   | 1:28:A:LEU:H   | 9        | 0.27          |
| (1,253)  | 1:26:A:TYR:HE1  | 1:45:A:THR:H   | 4        | 0.27          |
| (1,253)  | 1:26:A:TYR:HE2  | 1:45:A:THR:H   | 4        | 0.27          |
| (1,225)  | 1:23:A:SER:H    | 1:25:A:GLY:H   | 13       | 0.27          |
| (1,116)  | 1:17:A:PHE:H    | 1:56:A:TRP:HD1 | 12       | 0.27          |
| (1,116)  | 1:17:A:PHE:H    | 1:56:A:TRP:HD1 | 17       | 0.27          |
| (1,1656) | 1:137:A:HIS:HE1 | 1:126:A:LYS:H  | 15       | 0.26          |
| (1,1525) | 1:158:A:VAL:HB  | 1:159:A:LEU:H  | 4        | 0.26          |
| (1,1525) | 1:158:A:VAL:HB  | 1:159:A:LEU:H  | 5        | 0.26          |
| (1,1525) | 1:158:A:VAL:HB  | 1:159:A:LEU:H  | 6        | 0.26          |
| (1,1525) | 1:158:A:VAL:HB  | 1:159:A:LEU:H  | 12       | 0.26          |
| (1,1525) | 1:158:A:VAL:HB  | 1:159:A:LEU:H  | 14       | 0.26          |
| (1,1485) | 1:152:A:GLU:H   | 1:154:A:ARG:H  | 6        | 0.26          |
| (1,1485) | 1:152:A:GLU:H   | 1:154:A:ARG:H  | 8        | 0.26          |
| (1,1485) | 1:152:A:GLU:H   | 1:154:A:ARG:H  | 12       | 0.26          |
| (1,1461) | 1:150:A:ARG:H   | 1:152:A:GLU:H  | 7        | 0.26          |
| (1,1461) | 1:150:A:ARG:H   | 1:152:A:GLU:H  | 8        | 0.26          |
| (1,1461) | 1:150:A:ARG:H   | 1:152:A:GLU:H  | 16       | 0.26          |
| (1,1442) | 1:149:A:ASP:HA  | 1:150:A:ARG:H  | 1        | 0.26          |
| (1,1442) | 1:149:A:ASP:HA  | 1:150:A:ARG:H  | 3        | 0.26          |
| (1,1405) | 1:145:A:LYS:HA  | 1:147:A:HIS:H  | 4        | 0.26          |
| (1,1402) | 1:144:A:ASP:H   | 1:145:A:LYS:H  | 5        | 0.26          |
| (1,1163) | 1:115:A:LEU:HG  | 1:120:A:SER:H  | 6        | 0.26          |
| (1,1163) | 1:115:A:LEU:HG  | 1:120:A:SER:H  | 11       | 0.26          |
| (1,1163) | 1:115:A:LEU:HG  | 1:120:A:SER:H  | 12       | 0.26          |
| (1,1163) | 1:115:A:LEU:HG  | 1:120:A:SER:H  | 17       | 0.26          |
| (1,1163) | 1:115:A:LEU:HG  | 1:120:A:SER:H  | 18       | 0.26          |
| (1,1161) | 1:115:A:LEU:HG  | 1:117:A:ASN:H  | 2        | 0.26          |
| (1,1073) | 1:106:A:GLY:H   | 1:114:A:TYR:H  | 11       | 0.26          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1018) | 1:100:A:LEU:HA  | 1:101:A:ASN:H  | 3        | 0.26          |
| (1,1018) | 1:100:A:LEU:HA  | 1:101:A:ASN:H  | 6        | 0.26          |
| (1,1018) | 1:100:A:LEU:HA  | 1:101:A:ASN:H  | 14       | 0.26          |
| (1,1018) | 1:100:A:LEU:HA  | 1:101:A:ASN:H  | 16       | 0.26          |
| (1,1018) | 1:100:A:LEU:HA  | 1:101:A:ASN:H  | 18       | 0.26          |
| (1,1016) | 1:99:A:ASP:H    | 1:101:A:ASN:H  | 1        | 0.26          |
| (1,1016) | 1:99:A:ASP:H    | 1:101:A:ASN:H  | 17       | 0.26          |
| (1,960)  | 1:95:A:ASN:HA   | 1:96:A:VAL:H   | 15       | 0.26          |
| (1,783)  | 1:75:A:ILE:HB   | 1:76:A:ALA:H   | 18       | 0.26          |
| (1,696)  | 1:66:A:ASN:H    | 1:70:A:GLY:H   | 10       | 0.26          |
| (1,500)  | 1:47:A:ARG:H    | 1:49:A:LYS:H   | 1        | 0.26          |
| (1,488)  | 1:47:A:ARG:HA   | 1:49:A:LYS:H   | 17       | 0.26          |
| (1,441)  | 1:43:A:LEU:HA   | 1:135:A:GLY:H  | 1        | 0.26          |
| (1,441)  | 1:43:A:LEU:HA   | 1:135:A:GLY:H  | 8        | 0.26          |
| (1,441)  | 1:43:A:LEU:HA   | 1:135:A:GLY:H  | 17       | 0.26          |
| (1,357)  | 1:34:A:SER:HA   | 1:36:A:GLU:H   | 1        | 0.26          |
| (1,357)  | 1:34:A:SER:HA   | 1:36:A:GLU:H   | 11       | 0.26          |
| (1,284)  | 1:28:A:LEU:HG   | 1:28:A:LEU:H   | 15       | 0.26          |
| (1,284)  | 1:28:A:LEU:HG   | 1:28:A:LEU:H   | 18       | 0.26          |
| (1,225)  | 1:23:A:SER:H    | 1:25:A:GLY:H   | 1        | 0.26          |
| (1,225)  | 1:23:A:SER:H    | 1:25:A:GLY:H   | 5        | 0.26          |
| (1,116)  | 1:17:A:PHE:H    | 1:56:A:TRP:HD1 | 9        | 0.26          |
| (1,1656) | 1:137:A:HIS:HE1 | 1:126:A:LYS:H  | 3        | 0.25          |
| (1,1656) | 1:137:A:HIS:HE1 | 1:126:A:LYS:H  | 8        | 0.25          |
| (1,1656) | 1:137:A:HIS:HE1 | 1:126:A:LYS:H  | 17       | 0.25          |
| (1,1525) | 1:158:A:VAL:HB  | 1:159:A:LEU:H  | 2        | 0.25          |
| (1,1525) | 1:158:A:VAL:HB  | 1:159:A:LEU:H  | 7        | 0.25          |
| (1,1485) | 1:152:A:GLU:H   | 1:154:A:ARG:H  | 19       | 0.25          |
| (1,1461) | 1:150:A:ARG:H   | 1:152:A:GLU:H  | 6        | 0.25          |
| (1,1155) | 1:115:A:LEU:HB2 | 1:118:A:LYS:H  | 14       | 0.25          |
| (1,1155) | 1:115:A:LEU:HB3 | 1:118:A:LYS:H  | 14       | 0.25          |
| (1,1018) | 1:100:A:LEU:HA  | 1:101:A:ASN:H  | 1        | 0.25          |
| (1,1018) | 1:100:A:LEU:HA  | 1:101:A:ASN:H  | 2        | 0.25          |
| (1,1016) | 1:99:A:ASP:H    | 1:101:A:ASN:H  | 3        | 0.25          |
| (1,1016) | 1:99:A:ASP:H    | 1:101:A:ASN:H  | 11       | 0.25          |
| (1,1016) | 1:99:A:ASP:H    | 1:101:A:ASN:H  | 14       | 0.25          |
| (1,1016) | 1:99:A:ASP:H    | 1:101:A:ASN:H  | 18       | 0.25          |
| (1,927)  | 1:90:A:THR:HB   | 1:91:A:GLN:H   | 10       | 0.25          |
| (1,601)  | 1:57:A:ARG:H    | 1:64:A:LEU:HA  | 17       | 0.25          |
| (1,500)  | 1:47:A:ARG:H    | 1:49:A:LYS:H   | 3        | 0.25          |
| (1,357)  | 1:34:A:SER:HA   | 1:36:A:GLU:H   | 19       | 0.25          |
| (1,284)  | 1:28:A:LEU:HG   | 1:28:A:LEU:H   | 3        | 0.25          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,284)  | 1:28:A:LEU:HG   | 1:28:A:LEU:H   | 17       | 0.25          |
| (1,284)  | 1:28:A:LEU:HG   | 1:28:A:LEU:H   | 19       | 0.25          |
| (1,253)  | 1:26:A:TYR:HE1  | 1:45:A:THR:H   | 14       | 0.25          |
| (1,253)  | 1:26:A:TYR:HE2  | 1:45:A:THR:H   | 14       | 0.25          |
| (1,116)  | 1:17:A:PHE:H    | 1:56:A:TRP:HD1 | 13       | 0.25          |
| (1,99)   | 1:16:A:TRP:HD1  | 1:17:A:PHE:H   | 3        | 0.25          |
| (1,98)   | 1:16:A:TRP:HD1  | 1:16:A:TRP:H   | 3        | 0.25          |
| (1,45)   | 1:9:A:SER:HA    | 1:107:A:LEU:H  | 10       | 0.25          |
| (1,29)   | 1:6:A:PHE:H     | 1:7:A:GLU:H    | 9        | 0.25          |
| (1,1525) | 1:158:A:VAL:HB  | 1:159:A:LEU:H  | 1        | 0.24          |
| (1,1525) | 1:158:A:VAL:HB  | 1:159:A:LEU:H  | 13       | 0.24          |
| (1,1525) | 1:158:A:VAL:HB  | 1:159:A:LEU:H  | 16       | 0.24          |
| (1,1525) | 1:158:A:VAL:HB  | 1:159:A:LEU:H  | 17       | 0.24          |
| (1,1485) | 1:152:A:GLU:H   | 1:154:A:ARG:H  | 9        | 0.24          |
| (1,1485) | 1:152:A:GLU:H   | 1:154:A:ARG:H  | 13       | 0.24          |
| (1,1461) | 1:150:A:ARG:H   | 1:152:A:GLU:H  | 5        | 0.24          |
| (1,1442) | 1:149:A:ASP:HA  | 1:150:A:ARG:H  | 4        | 0.24          |
| (1,1402) | 1:144:A:ASP:H   | 1:145:A:LYS:H  | 15       | 0.24          |
| (1,1321) | 1:133:A:ARG:HA  | 1:136:A:LEU:H  | 3        | 0.24          |
| (1,1163) | 1:115:A:LEU:HG  | 1:120:A:SER:H  | 19       | 0.24          |
| (1,1155) | 1:115:A:LEU:HB2 | 1:118:A:LYS:H  | 3        | 0.24          |
| (1,1155) | 1:115:A:LEU:HB3 | 1:118:A:LYS:H  | 3        | 0.24          |
| (1,1155) | 1:115:A:LEU:HB2 | 1:118:A:LYS:H  | 8        | 0.24          |
| (1,1155) | 1:115:A:LEU:HB3 | 1:118:A:LYS:H  | 8        | 0.24          |
| (1,1155) | 1:115:A:LEU:HB2 | 1:118:A:LYS:H  | 13       | 0.24          |
| (1,1155) | 1:115:A:LEU:HB3 | 1:118:A:LYS:H  | 13       | 0.24          |
| (1,1073) | 1:106:A:GLY:H   | 1:114:A:TYR:H  | 15       | 0.24          |
| (1,1018) | 1:100:A:LEU:HA  | 1:101:A:ASN:H  | 8        | 0.24          |
| (1,1018) | 1:100:A:LEU:HA  | 1:101:A:ASN:H  | 20       | 0.24          |
| (1,927)  | 1:90:A:THR:HB   | 1:91:A:GLN:H   | 6        | 0.24          |
| (1,927)  | 1:90:A:THR:HB   | 1:91:A:GLN:H   | 8        | 0.24          |
| (1,696)  | 1:66:A:ASN:H    | 1:70:A:GLY:H   | 11       | 0.24          |
| (1,696)  | 1:66:A:ASN:H    | 1:70:A:GLY:H   | 16       | 0.24          |
| (1,623)  | 1:59:A:ASP:H    | 1:63:A:TYR:HD1 | 1        | 0.24          |
| (1,441)  | 1:43:A:LEU:HA   | 1:135:A:GLY:H  | 11       | 0.24          |
| (1,305)  | 1:29:A:MET:H    | 1:42:A:VAL:H   | 10       | 0.24          |
| (1,291)  | 1:29:A:MET:HA   | 1:56:A:TRP:HE1 | 15       | 0.24          |
| (1,285)  | 1:28:A:LEU:HG   | 1:29:A:MET:H   | 5        | 0.24          |
| (1,284)  | 1:28:A:LEU:HG   | 1:28:A:LEU:H   | 4        | 0.24          |
| (1,284)  | 1:28:A:LEU:HG   | 1:28:A:LEU:H   | 8        | 0.24          |
| (1,284)  | 1:28:A:LEU:HG   | 1:28:A:LEU:H   | 11       | 0.24          |
| (1,225)  | 1:23:A:SER:H    | 1:25:A:GLY:H   | 2        | 0.24          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,116)  | 1:17:A:PHE:H    | 1:56:A:TRP:HD1 | 8        | 0.24          |
| (1,116)  | 1:17:A:PHE:H    | 1:56:A:TRP:HD1 | 10       | 0.24          |
| (1,45)   | 1:9:A:SER:HA    | 1:107:A:LEU:H  | 15       | 0.24          |
| (1,1485) | 1:152:A:GLU:H   | 1:154:A:ARG:H  | 5        | 0.23          |
| (1,1485) | 1:152:A:GLU:H   | 1:154:A:ARG:H  | 10       | 0.23          |
| (1,1461) | 1:150:A:ARG:H   | 1:152:A:GLU:H  | 19       | 0.23          |
| (1,1442) | 1:149:A:ASP:HA  | 1:150:A:ARG:H  | 5        | 0.23          |
| (1,1405) | 1:145:A:LYS:HA  | 1:147:A:HIS:H  | 7        | 0.23          |
| (1,1402) | 1:144:A:ASP:H   | 1:145:A:LYS:H  | 8        | 0.23          |
| (1,1402) | 1:144:A:ASP:H   | 1:145:A:LYS:H  | 11       | 0.23          |
| (1,1402) | 1:144:A:ASP:H   | 1:145:A:LYS:H  | 13       | 0.23          |
| (1,1402) | 1:144:A:ASP:H   | 1:145:A:LYS:H  | 19       | 0.23          |
| (1,1364) | 1:139:A:HIS:HD2 | 1:139:A:HIS:H  | 16       | 0.23          |
| (1,1321) | 1:133:A:ARG:HA  | 1:136:A:LEU:H  | 18       | 0.23          |
| (1,1318) | 1:132:A:ARG:HG2 | 1:134:A:GLU:H  | 20       | 0.23          |
| (1,1318) | 1:132:A:ARG:HG3 | 1:134:A:GLU:H  | 20       | 0.23          |
| (1,1163) | 1:115:A:LEU:HG  | 1:120:A:SER:H  | 5        | 0.23          |
| (1,1163) | 1:115:A:LEU:HG  | 1:120:A:SER:H  | 15       | 0.23          |
| (1,1163) | 1:115:A:LEU:HG  | 1:120:A:SER:H  | 20       | 0.23          |
| (1,1155) | 1:115:A:LEU:HB2 | 1:118:A:LYS:H  | 6        | 0.23          |
| (1,1155) | 1:115:A:LEU:HB3 | 1:118:A:LYS:H  | 6        | 0.23          |
| (1,1155) | 1:115:A:LEU:HB2 | 1:118:A:LYS:H  | 15       | 0.23          |
| (1,1155) | 1:115:A:LEU:HB3 | 1:118:A:LYS:H  | 15       | 0.23          |
| (1,1155) | 1:115:A:LEU:HB2 | 1:118:A:LYS:H  | 16       | 0.23          |
| (1,1155) | 1:115:A:LEU:HB3 | 1:118:A:LYS:H  | 16       | 0.23          |
| (1,1155) | 1:115:A:LEU:HB2 | 1:118:A:LYS:H  | 19       | 0.23          |
| (1,1155) | 1:115:A:LEU:HB3 | 1:118:A:LYS:H  | 19       | 0.23          |
| (1,1073) | 1:106:A:GLY:H   | 1:114:A:TYR:H  | 9        | 0.23          |
| (1,1073) | 1:106:A:GLY:H   | 1:114:A:TYR:H  | 16       | 0.23          |
| (1,1016) | 1:99:A:ASP:H    | 1:101:A:ASN:H  | 2        | 0.23          |
| (1,1016) | 1:99:A:ASP:H    | 1:101:A:ASN:H  | 4        | 0.23          |
| (1,1016) | 1:99:A:ASP:H    | 1:101:A:ASN:H  | 6        | 0.23          |
| (1,960)  | 1:95:A:ASN:HA   | 1:96:A:VAL:H   | 17       | 0.23          |
| (1,960)  | 1:95:A:ASN:HA   | 1:96:A:VAL:H   | 19       | 0.23          |
| (1,927)  | 1:90:A:THR:HB   | 1:91:A:GLN:H   | 2        | 0.23          |
| (1,927)  | 1:90:A:THR:HB   | 1:91:A:GLN:H   | 4        | 0.23          |
| (1,728)  | 1:69:A:SER:H    | 1:71:A:GLN:H   | 20       | 0.23          |
| (1,629)  | 1:60:A:PRO:HA   | 1:62:A:GLY:H   | 16       | 0.23          |
| (1,623)  | 1:59:A:ASP:H    | 1:63:A:TYR:HD1 | 4        | 0.23          |
| (1,570)  | 1:55:A:LEU:H    | 1:56:A:TRP:HE1 | 5        | 0.23          |
| (1,441)  | 1:43:A:LEU:HA   | 1:135:A:GLY:H  | 3        | 0.23          |
| (1,441)  | 1:43:A:LEU:HA   | 1:135:A:GLY:H  | 5        | 0.23          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,441)  | 1:43:A:LEU:HA   | 1:135:A:GLY:H  | 18       | 0.23          |
| (1,441)  | 1:43:A:LEU:HA   | 1:135:A:GLY:H  | 20       | 0.23          |
| (1,357)  | 1:34:A:SER:HA   | 1:36:A:GLU:H   | 3        | 0.23          |
| (1,305)  | 1:29:A:MET:H    | 1:42:A:VAL:H   | 1        | 0.23          |
| (1,284)  | 1:28:A:LEU:HG   | 1:28:A:LEU:H   | 2        | 0.23          |
| (1,253)  | 1:26:A:TYR:HE1  | 1:45:A:THR:H   | 16       | 0.23          |
| (1,253)  | 1:26:A:TYR:HE2  | 1:45:A:THR:H   | 16       | 0.23          |
| (1,253)  | 1:26:A:TYR:HE1  | 1:45:A:THR:H   | 20       | 0.23          |
| (1,253)  | 1:26:A:TYR:HE2  | 1:45:A:THR:H   | 20       | 0.23          |
| (1,225)  | 1:23:A:SER:H    | 1:25:A:GLY:H   | 4        | 0.23          |
| (1,116)  | 1:17:A:PHE:H    | 1:56:A:TRP:HD1 | 16       | 0.23          |
| (1,116)  | 1:17:A:PHE:H    | 1:56:A:TRP:HD1 | 20       | 0.23          |
| (1,45)   | 1:9:A:SER:HA    | 1:107:A:LEU:H  | 8        | 0.23          |
| (1,29)   | 1:6:A:PHE:H     | 1:7:A:GLU:H    | 13       | 0.23          |
| (1,7)    | 1:4:A:ALA:HA    | 1:6:A:PHE:H    | 6        | 0.23          |
| (1,1656) | 1:137:A:HIS:HE1 | 1:126:A:LYS:H  | 7        | 0.22          |
| (1,1485) | 1:152:A:GLU:H   | 1:154:A:ARG:H  | 15       | 0.22          |
| (1,1485) | 1:152:A:GLU:H   | 1:154:A:ARG:H  | 18       | 0.22          |
| (1,1485) | 1:152:A:GLU:H   | 1:154:A:ARG:H  | 20       | 0.22          |
| (1,1461) | 1:150:A:ARG:H   | 1:152:A:GLU:H  | 12       | 0.22          |
| (1,1402) | 1:144:A:ASP:H   | 1:145:A:LYS:H  | 2        | 0.22          |
| (1,1402) | 1:144:A:ASP:H   | 1:145:A:LYS:H  | 10       | 0.22          |
| (1,1163) | 1:115:A:LEU:HG  | 1:120:A:SER:H  | 1        | 0.22          |
| (1,1163) | 1:115:A:LEU:HG  | 1:120:A:SER:H  | 16       | 0.22          |
| (1,1161) | 1:115:A:LEU:HG  | 1:117:A:ASN:H  | 5        | 0.22          |
| (1,1161) | 1:115:A:LEU:HG  | 1:117:A:ASN:H  | 9        | 0.22          |
| (1,1155) | 1:115:A:LEU:HB2 | 1:118:A:LYS:H  | 1        | 0.22          |
| (1,1155) | 1:115:A:LEU:HB3 | 1:118:A:LYS:H  | 1        | 0.22          |
| (1,1155) | 1:115:A:LEU:HB2 | 1:118:A:LYS:H  | 4        | 0.22          |
| (1,1155) | 1:115:A:LEU:HB3 | 1:118:A:LYS:H  | 4        | 0.22          |
| (1,1155) | 1:115:A:LEU:HB2 | 1:118:A:LYS:H  | 11       | 0.22          |
| (1,1155) | 1:115:A:LEU:HB3 | 1:118:A:LYS:H  | 11       | 0.22          |
| (1,1155) | 1:115:A:LEU:HB2 | 1:118:A:LYS:H  | 12       | 0.22          |
| (1,1155) | 1:115:A:LEU:HB3 | 1:118:A:LYS:H  | 12       | 0.22          |
| (1,1155) | 1:115:A:LEU:HB2 | 1:118:A:LYS:H  | 17       | 0.22          |
| (1,1155) | 1:115:A:LEU:HB3 | 1:118:A:LYS:H  | 17       | 0.22          |
| (1,1155) | 1:115:A:LEU:HB2 | 1:118:A:LYS:H  | 18       | 0.22          |
| (1,1155) | 1:115:A:LEU:HB3 | 1:118:A:LYS:H  | 18       | 0.22          |
| (1,1080) | 1:107:A:LEU:HA  | 1:114:A:TYR:H  | 11       | 0.22          |
| (1,1073) | 1:106:A:GLY:H   | 1:114:A:TYR:H  | 10       | 0.22          |
| (1,1018) | 1:100:A:LEU:HA  | 1:101:A:ASN:H  | 11       | 0.22          |
| (1,1016) | 1:99:A:ASP:H    | 1:101:A:ASN:H  | 9        | 0.22          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,960)  | 1:95:A:ASN:HA   | 1:96:A:VAL:H   | 6        | 0.22          |
| (1,960)  | 1:95:A:ASN:HA   | 1:96:A:VAL:H   | 8        | 0.22          |
| (1,960)  | 1:95:A:ASN:HA   | 1:96:A:VAL:H   | 9        | 0.22          |
| (1,927)  | 1:90:A:THR:HB   | 1:91:A:GLN:H   | 15       | 0.22          |
| (1,881)  | 1:84:A:VAL:H    | 1:140:A:LEU:H  | 19       | 0.22          |
| (1,783)  | 1:75:A:ILE:HB   | 1:76:A:ALA:H   | 16       | 0.22          |
| (1,783)  | 1:75:A:ILE:HB   | 1:76:A:ALA:H   | 20       | 0.22          |
| (1,696)  | 1:66:A:ASN:H    | 1:70:A:GLY:H   | 12       | 0.22          |
| (1,696)  | 1:66:A:ASN:H    | 1:70:A:GLY:H   | 13       | 0.22          |
| (1,623)  | 1:59:A:ASP:H    | 1:63:A:TYR:HD1 | 13       | 0.22          |
| (1,623)  | 1:59:A:ASP:H    | 1:63:A:TYR:HD1 | 18       | 0.22          |
| (1,608)  | 1:58:A:HIS:HA   | 1:65:A:VAL:H   | 17       | 0.22          |
| (1,500)  | 1:47:A:ARG:H    | 1:49:A:LYS:H   | 8        | 0.22          |
| (1,441)  | 1:43:A:LEU:HA   | 1:135:A:GLY:H  | 6        | 0.22          |
| (1,441)  | 1:43:A:LEU:HA   | 1:135:A:GLY:H  | 15       | 0.22          |
| (1,441)  | 1:43:A:LEU:HA   | 1:135:A:GLY:H  | 16       | 0.22          |
| (1,363)  | 1:34:A:SER:H    | 1:36:A:GLU:H   | 5        | 0.22          |
| (1,357)  | 1:34:A:SER:HA   | 1:36:A:GLU:H   | 9        | 0.22          |
| (1,317)  | 1:30:A:VAL:HG11 | 1:34:A:SER:H   | 10       | 0.22          |
| (1,317)  | 1:30:A:VAL:HG12 | 1:34:A:SER:H   | 10       | 0.22          |
| (1,317)  | 1:30:A:VAL:HG13 | 1:34:A:SER:H   | 10       | 0.22          |
| (1,317)  | 1:30:A:VAL:HG21 | 1:34:A:SER:H   | 10       | 0.22          |
| (1,317)  | 1:30:A:VAL:HG22 | 1:34:A:SER:H   | 10       | 0.22          |
| (1,317)  | 1:30:A:VAL:HG23 | 1:34:A:SER:H   | 10       | 0.22          |
| (1,284)  | 1:28:A:LEU:HG   | 1:28:A:LEU:H   | 10       | 0.22          |
| (1,284)  | 1:28:A:LEU:HG   | 1:28:A:LEU:H   | 14       | 0.22          |
| (1,253)  | 1:26:A:TYR:HE1  | 1:45:A:THR:H   | 1        | 0.22          |
| (1,253)  | 1:26:A:TYR:HE2  | 1:45:A:THR:H   | 1        | 0.22          |
| (1,253)  | 1:26:A:TYR:HE1  | 1:45:A:THR:H   | 7        | 0.22          |
| (1,253)  | 1:26:A:TYR:HE2  | 1:45:A:THR:H   | 7        | 0.22          |
| (1,225)  | 1:23:A:SER:H    | 1:25:A:GLY:H   | 11       | 0.22          |
| (1,223)  | 1:23:A:SER:H    | 1:152:A:GLU:H  | 18       | 0.22          |
| (1,45)   | 1:9:A:SER:HA    | 1:107:A:LEU:H  | 9        | 0.22          |
| (1,45)   | 1:9:A:SER:HA    | 1:107:A:LEU:H  | 19       | 0.22          |
| (1,29)   | 1:6:A:PHE:H     | 1:7:A:GLU:H    | 16       | 0.22          |
| (1,1539) | 1:161:A:VAL:HB  | 1:161:A:VAL:H  | 4        | 0.21          |
| (1,1485) | 1:152:A:GLU:H   | 1:154:A:ARG:H  | 17       | 0.21          |
| (1,1461) | 1:150:A:ARG:H   | 1:152:A:GLU:H  | 2        | 0.21          |
| (1,1442) | 1:149:A:ASP:HA  | 1:150:A:ARG:H  | 7        | 0.21          |
| (1,1442) | 1:149:A:ASP:HA  | 1:150:A:ARG:H  | 8        | 0.21          |
| (1,1442) | 1:149:A:ASP:HA  | 1:150:A:ARG:H  | 20       | 0.21          |
| (1,1405) | 1:145:A:LYS:HA  | 1:147:A:HIS:H  | 10       | 0.21          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1402) | 1:144:A:ASP:H    | 1:145:A:LYS:H   | 6        | 0.21          |
| (1,1364) | 1:139:A:HIS:HD2  | 1:139:A:HIS:H   | 20       | 0.21          |
| (1,1321) | 1:133:A:ARG:HA   | 1:136:A:LEU:H   | 9        | 0.21          |
| (1,1321) | 1:133:A:ARG:HA   | 1:136:A:LEU:H   | 11       | 0.21          |
| (1,1310) | 1:132:A:ARG:HA   | 1:134:A:GLU:H   | 3        | 0.21          |
| (1,1163) | 1:115:A:LEU:HG   | 1:120:A:SER:H   | 9        | 0.21          |
| (1,1161) | 1:115:A:LEU:HG   | 1:117:A:ASN:H   | 7        | 0.21          |
| (1,1155) | 1:115:A:LEU:HB2  | 1:118:A:LYS:H   | 20       | 0.21          |
| (1,1155) | 1:115:A:LEU:HB3  | 1:118:A:LYS:H   | 20       | 0.21          |
| (1,1073) | 1:106:A:GLY:H    | 1:114:A:TYR:H   | 4        | 0.21          |
| (1,968)  | 1:96:A:VAL:HB    | 1:96:A:VAL:H    | 18       | 0.21          |
| (1,960)  | 1:95:A:ASN:HA    | 1:96:A:VAL:H    | 10       | 0.21          |
| (1,927)  | 1:90:A:THR:HB    | 1:91:A:GLN:H    | 14       | 0.21          |
| (1,696)  | 1:66:A:ASN:H     | 1:70:A:GLY:H    | 7        | 0.21          |
| (1,696)  | 1:66:A:ASN:H     | 1:70:A:GLY:H    | 19       | 0.21          |
| (1,623)  | 1:59:A:ASP:H     | 1:63:A:TYR:HD1  | 10       | 0.21          |
| (1,608)  | 1:58:A:HIS:HA    | 1:65:A:VAL:H    | 5        | 0.21          |
| (1,441)  | 1:43:A:LEU:HA    | 1:135:A:GLY:H   | 2        | 0.21          |
| (1,441)  | 1:43:A:LEU:HA    | 1:135:A:GLY:H   | 4        | 0.21          |
| (1,441)  | 1:43:A:LEU:HA    | 1:135:A:GLY:H   | 9        | 0.21          |
| (1,441)  | 1:43:A:LEU:HA    | 1:135:A:GLY:H   | 13       | 0.21          |
| (1,357)  | 1:34:A:SER:HA    | 1:36:A:GLU:H    | 10       | 0.21          |
| (1,317)  | 1:30:A:VAL:HG11  | 1:34:A:SER:H    | 1        | 0.21          |
| (1,317)  | 1:30:A:VAL:HG12  | 1:34:A:SER:H    | 1        | 0.21          |
| (1,317)  | 1:30:A:VAL:HG13  | 1:34:A:SER:H    | 1        | 0.21          |
| (1,317)  | 1:30:A:VAL:HG21  | 1:34:A:SER:H    | 1        | 0.21          |
| (1,317)  | 1:30:A:VAL:HG22  | 1:34:A:SER:H    | 1        | 0.21          |
| (1,317)  | 1:30:A:VAL:HG23  | 1:34:A:SER:H    | 1        | 0.21          |
| (1,300)  | 1:29:A:MET:HG2   | 1:30:A:VAL:H    | 12       | 0.21          |
| (1,300)  | 1:29:A:MET:HG3   | 1:30:A:VAL:H    | 12       | 0.21          |
| (1,223)  | 1:23:A:SER:H     | 1:152:A:GLU:H   | 17       | 0.21          |
| (1,210)  | 1:22:A:ASN:H     | 1:156:A:ASP:H   | 6        | 0.21          |
| (1,195)  | 1:21:A:ASN:H     | 1:155:A:TRP:HH2 | 9        | 0.21          |
| (1,116)  | 1:17:A:PHE:H     | 1:56:A:TRP:HD1  | 6        | 0.21          |
| (1,115)  | 1:17:A:PHE:H     | 1:56:A:TRP:HA   | 15       | 0.21          |
| (1,45)   | 1:9:A:SER:HA     | 1:107:A:LEU:H   | 4        | 0.21          |
| (1,1639) | 1:115:A:LEU:HD11 | 1:118:A:LYS:HB2 | 4        | 0.2           |
| (1,1639) | 1:115:A:LEU:HD11 | 1:118:A:LYS:HB3 | 4        | 0.2           |
| (1,1639) | 1:115:A:LEU:HD12 | 1:118:A:LYS:HB2 | 4        | 0.2           |
| (1,1639) | 1:115:A:LEU:HD12 | 1:118:A:LYS:HB3 | 4        | 0.2           |
| (1,1639) | 1:115:A:LEU:HD13 | 1:118:A:LYS:HB2 | 4        | 0.2           |
| (1,1639) | 1:115:A:LEU:HD13 | 1:118:A:LYS:HB3 | 4        | 0.2           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1639) | 1:115:A:LEU:HD21 | 1:118:A:LYS:HB2 | 4        | 0.2           |
| (1,1639) | 1:115:A:LEU:HD21 | 1:118:A:LYS:HB3 | 4        | 0.2           |
| (1,1639) | 1:115:A:LEU:HD22 | 1:118:A:LYS:HB2 | 4        | 0.2           |
| (1,1639) | 1:115:A:LEU:HD22 | 1:118:A:LYS:HB3 | 4        | 0.2           |
| (1,1639) | 1:115:A:LEU:HD23 | 1:118:A:LYS:HB2 | 4        | 0.2           |
| (1,1639) | 1:115:A:LEU:HD23 | 1:118:A:LYS:HB3 | 4        | 0.2           |
| (1,1639) | 1:115:A:LEU:HD11 | 1:118:A:LYS:HB2 | 18       | 0.2           |
| (1,1639) | 1:115:A:LEU:HD11 | 1:118:A:LYS:HB3 | 18       | 0.2           |
| (1,1639) | 1:115:A:LEU:HD12 | 1:118:A:LYS:HB2 | 18       | 0.2           |
| (1,1639) | 1:115:A:LEU:HD12 | 1:118:A:LYS:HB3 | 18       | 0.2           |
| (1,1639) | 1:115:A:LEU:HD13 | 1:118:A:LYS:HB2 | 18       | 0.2           |
| (1,1639) | 1:115:A:LEU:HD13 | 1:118:A:LYS:HB3 | 18       | 0.2           |
| (1,1639) | 1:115:A:LEU:HD21 | 1:118:A:LYS:HB2 | 18       | 0.2           |
| (1,1639) | 1:115:A:LEU:HD21 | 1:118:A:LYS:HB3 | 18       | 0.2           |
| (1,1639) | 1:115:A:LEU:HD22 | 1:118:A:LYS:HB2 | 18       | 0.2           |
| (1,1639) | 1:115:A:LEU:HD22 | 1:118:A:LYS:HB3 | 18       | 0.2           |
| (1,1639) | 1:115:A:LEU:HD23 | 1:118:A:LYS:HB2 | 18       | 0.2           |
| (1,1639) | 1:115:A:LEU:HD23 | 1:118:A:LYS:HB3 | 18       | 0.2           |
| (1,1539) | 1:161:A:VAL:HB   | 1:161:A:VAL:H   | 1        | 0.2           |
| (1,1539) | 1:161:A:VAL:HB   | 1:161:A:VAL:H   | 18       | 0.2           |
| (1,1485) | 1:152:A:GLU:H    | 1:154:A:ARG:H   | 7        | 0.2           |
| (1,1431) | 1:147:A:HIS:H    | 1:148:A:LEU:HG  | 16       | 0.2           |
| (1,1321) | 1:133:A:ARG:HA   | 1:136:A:LEU:H   | 1        | 0.2           |
| (1,1321) | 1:133:A:ARG:HA   | 1:136:A:LEU:H   | 20       | 0.2           |
| (1,1163) | 1:115:A:LEU:HG   | 1:120:A:SER:H   | 10       | 0.2           |
| (1,1161) | 1:115:A:LEU:HG   | 1:117:A:ASN:H   | 10       | 0.2           |
| (1,1016) | 1:99:A:ASP:H     | 1:101:A:ASN:H   | 8        | 0.2           |
| (1,1016) | 1:99:A:ASP:H     | 1:101:A:ASN:H   | 12       | 0.2           |
| (1,960)  | 1:95:A:ASN:HA    | 1:96:A:VAL:H    | 20       | 0.2           |
| (1,927)  | 1:90:A:THR:HB    | 1:91:A:GLN:H    | 19       | 0.2           |
| (1,881)  | 1:84:A:VAL:H     | 1:140:A:LEU:H   | 13       | 0.2           |
| (1,783)  | 1:75:A:ILE:HB    | 1:76:A:ALA:H    | 8        | 0.2           |
| (1,783)  | 1:75:A:ILE:HB    | 1:76:A:ALA:H    | 13       | 0.2           |
| (1,745)  | 1:72:A:VAL:HB    | 1:73:A:MET:H    | 13       | 0.2           |
| (1,728)  | 1:69:A:SER:H     | 1:71:A:GLN:H    | 6        | 0.2           |
| (1,696)  | 1:66:A:ASN:H     | 1:70:A:GLY:H    | 2        | 0.2           |
| (1,695)  | 1:66:A:ASN:H     | 1:69:A:SER:H    | 13       | 0.2           |
| (1,441)  | 1:43:A:LEU:HA    | 1:135:A:GLY:H   | 10       | 0.2           |
| (1,317)  | 1:30:A:VAL:HG11  | 1:34:A:SER:H    | 9        | 0.2           |
| (1,317)  | 1:30:A:VAL:HG12  | 1:34:A:SER:H    | 9        | 0.2           |
| (1,317)  | 1:30:A:VAL:HG13  | 1:34:A:SER:H    | 9        | 0.2           |
| (1,317)  | 1:30:A:VAL:HG21  | 1:34:A:SER:H    | 9        | 0.2           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,317)  | 1:30:A:VAL:HG22 | 1:34:A:SER:H     | 9        | 0.2           |
| (1,317)  | 1:30:A:VAL:HG23 | 1:34:A:SER:H     | 9        | 0.2           |
| (1,305)  | 1:29:A:MET:H    | 1:42:A:VAL:H     | 2        | 0.2           |
| (1,305)  | 1:29:A:MET:H    | 1:42:A:VAL:H     | 9        | 0.2           |
| (1,291)  | 1:29:A:MET:HA   | 1:56:A:TRP:HE1   | 4        | 0.2           |
| (1,291)  | 1:29:A:MET:HA   | 1:56:A:TRP:HE1   | 8        | 0.2           |
| (1,284)  | 1:28:A:LEU:HG   | 1:28:A:LEU:H     | 1        | 0.2           |
| (1,259)  | 1:27:A:VAL:HB   | 1:28:A:LEU:H     | 1        | 0.2           |
| (1,242)  | 1:26:A:TYR:HA   | 1:46:A:LEU:H     | 14       | 0.2           |
| (1,225)  | 1:23:A:SER:H    | 1:25:A:GLY:H     | 18       | 0.2           |
| (1,210)  | 1:22:A:ASN:H    | 1:156:A:ASP:H    | 8        | 0.2           |
| (1,210)  | 1:22:A:ASN:H    | 1:156:A:ASP:H    | 15       | 0.2           |
| (1,115)  | 1:17:A:PHE:H    | 1:56:A:TRP:HA    | 16       | 0.2           |
| (1,29)   | 1:6:A:PHE:H     | 1:7:A:GLU:H      | 4        | 0.2           |
| (1,7)    | 1:4:A:ALA:HA    | 1:6:A:PHE:H      | 8        | 0.2           |
| (1,7)    | 1:4:A:ALA:HA    | 1:6:A:PHE:H      | 17       | 0.2           |
| (1,1479) | 1:152:A:GLU:HA  | 1:154:A:ARG:H    | 11       | 0.19          |
| (1,1461) | 1:150:A:ARG:H   | 1:152:A:GLU:H    | 4        | 0.19          |
| (1,1461) | 1:150:A:ARG:H   | 1:152:A:GLU:H    | 11       | 0.19          |
| (1,1405) | 1:145:A:LYS:HA  | 1:147:A:HIS:H    | 14       | 0.19          |
| (1,1405) | 1:145:A:LYS:HA  | 1:147:A:HIS:H    | 19       | 0.19          |
| (1,1364) | 1:139:A:HIS:HD2 | 1:139:A:HIS:H    | 5        | 0.19          |
| (1,1321) | 1:133:A:ARG:HA  | 1:136:A:LEU:H    | 4        | 0.19          |
| (1,1321) | 1:133:A:ARG:HA  | 1:136:A:LEU:H    | 15       | 0.19          |
| (1,1294) | 1:129:A:PHE:HA  | 1:131:A:ALA:H    | 5        | 0.19          |
| (1,1163) | 1:115:A:LEU:HG  | 1:120:A:SER:H    | 7        | 0.19          |
| (1,1097) | 1:108:A:SER:H   | 1:114:A:TYR:HE1  | 16       | 0.19          |
| (1,1073) | 1:106:A:GLY:H   | 1:114:A:TYR:H    | 1        | 0.19          |
| (1,1016) | 1:99:A:ASP:H    | 1:101:A:ASN:H    | 16       | 0.19          |
| (1,970)  | 1:96:A:VAL:HG11 | 1:101:A:ASN:HD21 | 11       | 0.19          |
| (1,970)  | 1:96:A:VAL:HG11 | 1:101:A:ASN:HD22 | 11       | 0.19          |
| (1,970)  | 1:96:A:VAL:HG12 | 1:101:A:ASN:HD21 | 11       | 0.19          |
| (1,970)  | 1:96:A:VAL:HG12 | 1:101:A:ASN:HD22 | 11       | 0.19          |
| (1,970)  | 1:96:A:VAL:HG13 | 1:101:A:ASN:HD21 | 11       | 0.19          |
| (1,970)  | 1:96:A:VAL:HG13 | 1:101:A:ASN:HD22 | 11       | 0.19          |
| (1,970)  | 1:96:A:VAL:HG21 | 1:101:A:ASN:HD21 | 11       | 0.19          |
| (1,970)  | 1:96:A:VAL:HG21 | 1:101:A:ASN:HD22 | 11       | 0.19          |
| (1,970)  | 1:96:A:VAL:HG22 | 1:101:A:ASN:HD21 | 11       | 0.19          |
| (1,970)  | 1:96:A:VAL:HG22 | 1:101:A:ASN:HD22 | 11       | 0.19          |
| (1,970)  | 1:96:A:VAL:HG23 | 1:101:A:ASN:HD21 | 11       | 0.19          |
| (1,970)  | 1:96:A:VAL:HG23 | 1:101:A:ASN:HD22 | 11       | 0.19          |
| (1,968)  | 1:96:A:VAL:HB   | 1:96:A:VAL:H     | 16       | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,960)  | 1:95:A:ASN:HA   | 1:96:A:VAL:H    | 3        | 0.19          |
| (1,927)  | 1:90:A:THR:HB   | 1:91:A:GLN:H    | 12       | 0.19          |
| (1,881)  | 1:84:A:VAL:H    | 1:140:A:LEU:H   | 2        | 0.19          |
| (1,881)  | 1:84:A:VAL:H    | 1:140:A:LEU:H   | 10       | 0.19          |
| (1,783)  | 1:75:A:ILE:HB   | 1:76:A:ALA:H    | 6        | 0.19          |
| (1,647)  | 1:62:A:GLY:H    | 1:63:A:TYR:HD1  | 8        | 0.19          |
| (1,647)  | 1:62:A:GLY:H    | 1:63:A:TYR:HD1  | 12       | 0.19          |
| (1,629)  | 1:60:A:PRO:HA   | 1:62:A:GLY:H    | 14       | 0.19          |
| (1,608)  | 1:58:A:HIS:HA   | 1:65:A:VAL:H    | 10       | 0.19          |
| (1,608)  | 1:58:A:HIS:HA   | 1:65:A:VAL:H    | 11       | 0.19          |
| (1,603)  | 1:57:A:ARG:H    | 1:65:A:VAL:HB   | 1        | 0.19          |
| (1,500)  | 1:47:A:ARG:H    | 1:49:A:LYS:H    | 7        | 0.19          |
| (1,441)  | 1:43:A:LEU:HA   | 1:135:A:GLY:H   | 19       | 0.19          |
| (1,357)  | 1:34:A:SER:HA   | 1:36:A:GLU:H    | 5        | 0.19          |
| (1,223)  | 1:23:A:SER:H    | 1:152:A:GLU:H   | 15       | 0.19          |
| (1,116)  | 1:17:A:PHE:H    | 1:56:A:TRP:HD1  | 1        | 0.19          |
| (1,115)  | 1:17:A:PHE:H    | 1:56:A:TRP:HA   | 9        | 0.19          |
| (1,98)   | 1:16:A:TRP:HD1  | 1:16:A:TRP:H    | 4        | 0.19          |
| (1,98)   | 1:16:A:TRP:HD1  | 1:16:A:TRP:H    | 5        | 0.19          |
| (1,98)   | 1:16:A:TRP:HD1  | 1:16:A:TRP:H    | 14       | 0.19          |
| (1,1442) | 1:149:A:ASP:HA  | 1:150:A:ARG:H   | 6        | 0.18          |
| (1,1442) | 1:149:A:ASP:HA  | 1:150:A:ARG:H   | 10       | 0.18          |
| (1,1442) | 1:149:A:ASP:HA  | 1:150:A:ARG:H   | 11       | 0.18          |
| (1,1442) | 1:149:A:ASP:HA  | 1:150:A:ARG:H   | 18       | 0.18          |
| (1,1442) | 1:149:A:ASP:HA  | 1:150:A:ARG:H   | 19       | 0.18          |
| (1,1402) | 1:144:A:ASP:H   | 1:145:A:LYS:H   | 20       | 0.18          |
| (1,1356) | 1:138:A:VAL:HB  | 1:138:A:VAL:H   | 2        | 0.18          |
| (1,1345) | 1:136:A:LEU:HG  | 1:136:A:LEU:H   | 2        | 0.18          |
| (1,1321) | 1:133:A:ARG:HA  | 1:136:A:LEU:H   | 8        | 0.18          |
| (1,1318) | 1:132:A:ARG:HG2 | 1:134:A:GLU:H   | 7        | 0.18          |
| (1,1318) | 1:132:A:ARG:HG3 | 1:134:A:GLU:H   | 7        | 0.18          |
| (1,1318) | 1:132:A:ARG:HG2 | 1:134:A:GLU:H   | 9        | 0.18          |
| (1,1318) | 1:132:A:ARG:HG3 | 1:134:A:GLU:H   | 9        | 0.18          |
| (1,1310) | 1:132:A:ARG:HA  | 1:134:A:GLU:H   | 20       | 0.18          |
| (1,1097) | 1:108:A:SER:H   | 1:114:A:TYR:HE1 | 7        | 0.18          |
| (1,1080) | 1:107:A:LEU:HA  | 1:114:A:TYR:H   | 7        | 0.18          |
| (1,1073) | 1:106:A:GLY:H   | 1:114:A:TYR:H   | 19       | 0.18          |
| (1,960)  | 1:95:A:ASN:HA   | 1:96:A:VAL:H    | 13       | 0.18          |
| (1,927)  | 1:90:A:THR:HB   | 1:91:A:GLN:H    | 3        | 0.18          |
| (1,927)  | 1:90:A:THR:HB   | 1:91:A:GLN:H    | 5        | 0.18          |
| (1,881)  | 1:84:A:VAL:H    | 1:140:A:LEU:H   | 17       | 0.18          |
| (1,783)  | 1:75:A:ILE:HB   | 1:76:A:ALA:H    | 9        | 0.18          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,783)  | 1:75:A:ILE:HB    | 1:76:A:ALA:H    | 10       | 0.18          |
| (1,783)  | 1:75:A:ILE:HB    | 1:76:A:ALA:H    | 17       | 0.18          |
| (1,728)  | 1:69:A:SER:H     | 1:71:A:GLN:H    | 14       | 0.18          |
| (1,696)  | 1:66:A:ASN:H     | 1:70:A:GLY:H    | 3        | 0.18          |
| (1,695)  | 1:66:A:ASN:H     | 1:69:A:SER:H    | 3        | 0.18          |
| (1,647)  | 1:62:A:GLY:H     | 1:63:A:TYR:HD1  | 16       | 0.18          |
| (1,629)  | 1:60:A:PRO:HA    | 1:62:A:GLY:H    | 11       | 0.18          |
| (1,623)  | 1:59:A:ASP:H     | 1:63:A:TYR:HD1  | 8        | 0.18          |
| (1,608)  | 1:58:A:HIS:HA    | 1:65:A:VAL:H    | 6        | 0.18          |
| (1,608)  | 1:58:A:HIS:HA    | 1:65:A:VAL:H    | 15       | 0.18          |
| (1,545)  | 1:53:A:SER:HA    | 1:68:A:LYS:H    | 18       | 0.18          |
| (1,500)  | 1:47:A:ARG:H     | 1:49:A:LYS:H    | 17       | 0.18          |
| (1,488)  | 1:47:A:ARG:HA    | 1:49:A:LYS:H    | 20       | 0.18          |
| (1,484)  | 1:46:A:LEU:HG    | 1:47:A:ARG:H    | 15       | 0.18          |
| (1,468)  | 1:45:A:THR:HB    | 1:46:A:LEU:H    | 8        | 0.18          |
| (1,468)  | 1:45:A:THR:HB    | 1:46:A:LEU:H    | 15       | 0.18          |
| (1,305)  | 1:29:A:MET:H     | 1:42:A:VAL:H    | 8        | 0.18          |
| (1,305)  | 1:29:A:MET:H     | 1:42:A:VAL:H    | 16       | 0.18          |
| (1,291)  | 1:29:A:MET:HA    | 1:56:A:TRP:HE1  | 1        | 0.18          |
| (1,225)  | 1:23:A:SER:H     | 1:25:A:GLY:H    | 20       | 0.18          |
| (1,116)  | 1:17:A:PHE:H     | 1:56:A:TRP:HD1  | 3        | 0.18          |
| (1,98)   | 1:16:A:TRP:HD1   | 1:16:A:TRP:H    | 18       | 0.18          |
| (1,29)   | 1:6:A:PHE:H      | 1:7:A:GLU:H     | 15       | 0.18          |
| (1,29)   | 1:6:A:PHE:H      | 1:7:A:GLU:H     | 20       | 0.18          |
| (1,1639) | 1:115:A:LEU:HD11 | 1:118:A:LYS:HB2 | 2        | 0.17          |
| (1,1639) | 1:115:A:LEU:HD11 | 1:118:A:LYS:HB3 | 2        | 0.17          |
| (1,1639) | 1:115:A:LEU:HD12 | 1:118:A:LYS:HB2 | 2        | 0.17          |
| (1,1639) | 1:115:A:LEU:HD12 | 1:118:A:LYS:HB3 | 2        | 0.17          |
| (1,1639) | 1:115:A:LEU:HD13 | 1:118:A:LYS:HB2 | 2        | 0.17          |
| (1,1639) | 1:115:A:LEU:HD13 | 1:118:A:LYS:HB3 | 2        | 0.17          |
| (1,1639) | 1:115:A:LEU:HD21 | 1:118:A:LYS:HB2 | 2        | 0.17          |
| (1,1639) | 1:115:A:LEU:HD21 | 1:118:A:LYS:HB3 | 2        | 0.17          |
| (1,1639) | 1:115:A:LEU:HD22 | 1:118:A:LYS:HB2 | 2        | 0.17          |
| (1,1639) | 1:115:A:LEU:HD22 | 1:118:A:LYS:HB3 | 2        | 0.17          |
| (1,1639) | 1:115:A:LEU:HD23 | 1:118:A:LYS:HB2 | 2        | 0.17          |
| (1,1639) | 1:115:A:LEU:HD23 | 1:118:A:LYS:HB3 | 2        | 0.17          |
| (1,1542) | 1:162:A:VAL:HB   | 1:162:A:VAL:H   | 2        | 0.17          |
| (1,1542) | 1:162:A:VAL:HB   | 1:162:A:VAL:H   | 3        | 0.17          |
| (1,1461) | 1:150:A:ARG:H    | 1:152:A:GLU:H   | 17       | 0.17          |
| (1,1442) | 1:149:A:ASP:HA   | 1:150:A:ARG:H   | 13       | 0.17          |
| (1,1442) | 1:149:A:ASP:HA   | 1:150:A:ARG:H   | 15       | 0.17          |
| (1,1405) | 1:145:A:LYS:HA   | 1:147:A:HIS:H   | 1        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1405) | 1:145:A:LYS:HA  | 1:147:A:HIS:H   | 11       | 0.17          |
| (1,1356) | 1:138:A:VAL:HB  | 1:138:A:VAL:H   | 1        | 0.17          |
| (1,1356) | 1:138:A:VAL:HB  | 1:138:A:VAL:H   | 4        | 0.17          |
| (1,1356) | 1:138:A:VAL:HB  | 1:138:A:VAL:H   | 10       | 0.17          |
| (1,1356) | 1:138:A:VAL:HB  | 1:138:A:VAL:H   | 17       | 0.17          |
| (1,1321) | 1:133:A:ARG:HA  | 1:136:A:LEU:H   | 7        | 0.17          |
| (1,1321) | 1:133:A:ARG:HA  | 1:136:A:LEU:H   | 16       | 0.17          |
| (1,1321) | 1:133:A:ARG:HA  | 1:136:A:LEU:H   | 19       | 0.17          |
| (1,1318) | 1:132:A:ARG:HG2 | 1:134:A:GLU:H   | 11       | 0.17          |
| (1,1318) | 1:132:A:ARG:HG3 | 1:134:A:GLU:H   | 11       | 0.17          |
| (1,1294) | 1:129:A:PHE:HA  | 1:131:A:ALA:H   | 13       | 0.17          |
| (1,1155) | 1:115:A:LEU:HB2 | 1:118:A:LYS:H   | 2        | 0.17          |
| (1,1155) | 1:115:A:LEU:HB3 | 1:118:A:LYS:H   | 2        | 0.17          |
| (1,1155) | 1:115:A:LEU:HB2 | 1:118:A:LYS:H   | 5        | 0.17          |
| (1,1155) | 1:115:A:LEU:HB3 | 1:118:A:LYS:H   | 5        | 0.17          |
| (1,1145) | 1:114:A:TYR:HD1 | 1:115:A:LEU:H   | 11       | 0.17          |
| (1,1097) | 1:108:A:SER:H   | 1:114:A:TYR:HE1 | 8        | 0.17          |
| (1,960)  | 1:95:A:ASN:HA   | 1:96:A:VAL:H    | 12       | 0.17          |
| (1,927)  | 1:90:A:THR:HB   | 1:91:A:GLN:H    | 9        | 0.17          |
| (1,927)  | 1:90:A:THR:HB   | 1:91:A:GLN:H    | 18       | 0.17          |
| (1,881)  | 1:84:A:VAL:H    | 1:140:A:LEU:H   | 16       | 0.17          |
| (1,783)  | 1:75:A:ILE:HB   | 1:76:A:ALA:H    | 1        | 0.17          |
| (1,783)  | 1:75:A:ILE:HB   | 1:76:A:ALA:H    | 7        | 0.17          |
| (1,783)  | 1:75:A:ILE:HB   | 1:76:A:ALA:H    | 12       | 0.17          |
| (1,745)  | 1:72:A:VAL:HB   | 1:73:A:MET:H    | 15       | 0.17          |
| (1,647)  | 1:62:A:GLY:H    | 1:63:A:TYR:HD1  | 2        | 0.17          |
| (1,647)  | 1:62:A:GLY:H    | 1:63:A:TYR:HD1  | 7        | 0.17          |
| (1,623)  | 1:59:A:ASP:H    | 1:63:A:TYR:HD1  | 20       | 0.17          |
| (1,603)  | 1:57:A:ARG:H    | 1:65:A:VAL:HB   | 13       | 0.17          |
| (1,603)  | 1:57:A:ARG:H    | 1:65:A:VAL:HB   | 15       | 0.17          |
| (1,570)  | 1:55:A:LEU:H    | 1:56:A:TRP:HE1  | 14       | 0.17          |
| (1,545)  | 1:53:A:SER:HA   | 1:68:A:LYS:H    | 15       | 0.17          |
| (1,488)  | 1:47:A:ARG:HA   | 1:49:A:LYS:H    | 4        | 0.17          |
| (1,483)  | 1:46:A:LEU:HG   | 1:46:A:LEU:H    | 14       | 0.17          |
| (1,453)  | 1:43:A:LEU:H    | 1:135:A:GLY:H   | 17       | 0.17          |
| (1,441)  | 1:43:A:LEU:HA   | 1:135:A:GLY:H   | 7        | 0.17          |
| (1,441)  | 1:43:A:LEU:HA   | 1:135:A:GLY:H   | 12       | 0.17          |
| (1,441)  | 1:43:A:LEU:HA   | 1:135:A:GLY:H   | 14       | 0.17          |
| (1,315)  | 1:30:A:VAL:HG11 | 1:31:A:ASP:H    | 9        | 0.17          |
| (1,315)  | 1:30:A:VAL:HG12 | 1:31:A:ASP:H    | 9        | 0.17          |
| (1,315)  | 1:30:A:VAL:HG13 | 1:31:A:ASP:H    | 9        | 0.17          |
| (1,315)  | 1:30:A:VAL:HG21 | 1:31:A:ASP:H    | 9        | 0.17          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,315)  | 1:30:A:VAL:HG22 | 1:31:A:ASP:H   | 9        | 0.17          |
| (1,315)  | 1:30:A:VAL:HG23 | 1:31:A:ASP:H   | 9        | 0.17          |
| (1,305)  | 1:29:A:MET:H    | 1:42:A:VAL:H   | 17       | 0.17          |
| (1,291)  | 1:29:A:MET:HA   | 1:56:A:TRP:HE1 | 3        | 0.17          |
| (1,291)  | 1:29:A:MET:HA   | 1:56:A:TRP:HE1 | 16       | 0.17          |
| (1,291)  | 1:29:A:MET:HA   | 1:56:A:TRP:HE1 | 17       | 0.17          |
| (1,286)  | 1:28:A:LEU:HG   | 1:56:A:TRP:HE1 | 14       | 0.17          |
| (1,285)  | 1:28:A:LEU:HG   | 1:29:A:MET:H   | 7        | 0.17          |
| (1,210)  | 1:22:A:ASN:H    | 1:156:A:ASP:H  | 10       | 0.17          |
| (1,175)  | 1:20:A:LYS:H    | 1:155:A:TRP:HA | 1        | 0.17          |
| (1,175)  | 1:20:A:LYS:H    | 1:155:A:TRP:HA | 9        | 0.17          |
| (1,115)  | 1:17:A:PHE:H    | 1:56:A:TRP:HA  | 19       | 0.17          |
| (1,98)   | 1:16:A:TRP:HD1  | 1:16:A:TRP:H   | 1        | 0.17          |
| (1,98)   | 1:16:A:TRP:HD1  | 1:16:A:TRP:H   | 6        | 0.17          |
| (1,98)   | 1:16:A:TRP:HD1  | 1:16:A:TRP:H   | 19       | 0.17          |
| (1,1485) | 1:152:A:GLU:H   | 1:154:A:ARG:H  | 3        | 0.16          |
| (1,1485) | 1:152:A:GLU:H   | 1:154:A:ARG:H  | 14       | 0.16          |
| (1,1405) | 1:145:A:LYS:HA  | 1:147:A:HIS:H  | 3        | 0.16          |
| (1,1405) | 1:145:A:LYS:HA  | 1:147:A:HIS:H  | 5        | 0.16          |
| (1,1405) | 1:145:A:LYS:HA  | 1:147:A:HIS:H  | 8        | 0.16          |
| (1,1405) | 1:145:A:LYS:HA  | 1:147:A:HIS:H  | 12       | 0.16          |
| (1,1405) | 1:145:A:LYS:HA  | 1:147:A:HIS:H  | 15       | 0.16          |
| (1,1402) | 1:144:A:ASP:H   | 1:145:A:LYS:H  | 16       | 0.16          |
| (1,1356) | 1:138:A:VAL:HB  | 1:138:A:VAL:H  | 8        | 0.16          |
| (1,1356) | 1:138:A:VAL:HB  | 1:138:A:VAL:H  | 14       | 0.16          |
| (1,1321) | 1:133:A:ARG:HA  | 1:136:A:LEU:H  | 12       | 0.16          |
| (1,1318) | 1:132:A:ARG:HG2 | 1:134:A:GLU:H  | 10       | 0.16          |
| (1,1318) | 1:132:A:ARG:HG3 | 1:134:A:GLU:H  | 10       | 0.16          |
| (1,1241) | 1:123:A:LEU:HG  | 1:123:A:LEU:H  | 6        | 0.16          |
| (1,1160) | 1:115:A:LEU:HG  | 1:116:A:ALA:H  | 1        | 0.16          |
| (1,1160) | 1:115:A:LEU:HG  | 1:116:A:ALA:H  | 16       | 0.16          |
| (1,940)  | 1:92:A:ALA:HA   | 1:93:A:GLY:H   | 2        | 0.16          |
| (1,927)  | 1:90:A:THR:HB   | 1:91:A:GLN:H   | 17       | 0.16          |
| (1,881)  | 1:84:A:VAL:H    | 1:140:A:LEU:H  | 5        | 0.16          |
| (1,881)  | 1:84:A:VAL:H    | 1:140:A:LEU:H  | 15       | 0.16          |
| (1,783)  | 1:75:A:ILE:HB   | 1:76:A:ALA:H   | 5        | 0.16          |
| (1,783)  | 1:75:A:ILE:HB   | 1:76:A:ALA:H   | 11       | 0.16          |
| (1,783)  | 1:75:A:ILE:HB   | 1:76:A:ALA:H   | 14       | 0.16          |
| (1,728)  | 1:69:A:SER:H    | 1:71:A:GLN:H   | 17       | 0.16          |
| (1,695)  | 1:66:A:ASN:H    | 1:69:A:SER:H   | 1        | 0.16          |
| (1,695)  | 1:66:A:ASN:H    | 1:69:A:SER:H   | 19       | 0.16          |
| (1,647)  | 1:62:A:GLY:H    | 1:63:A:TYR:HD1 | 14       | 0.16          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,623)  | 1:59:A:ASP:H     | 1:63:A:TYR:HD1  | 11       | 0.16          |
| (1,608)  | 1:58:A:HIS:HA    | 1:65:A:VAL:H    | 1        | 0.16          |
| (1,608)  | 1:58:A:HIS:HA    | 1:65:A:VAL:H    | 4        | 0.16          |
| (1,608)  | 1:58:A:HIS:HA    | 1:65:A:VAL:H    | 9        | 0.16          |
| (1,608)  | 1:58:A:HIS:HA    | 1:65:A:VAL:H    | 13       | 0.16          |
| (1,570)  | 1:55:A:LEU:H     | 1:56:A:TRP:HE1  | 4        | 0.16          |
| (1,570)  | 1:55:A:LEU:H     | 1:56:A:TRP:HE1  | 10       | 0.16          |
| (1,500)  | 1:47:A:ARG:H     | 1:49:A:LYS:H    | 15       | 0.16          |
| (1,468)  | 1:45:A:THR:HB    | 1:46:A:LEU:H    | 9        | 0.16          |
| (1,453)  | 1:43:A:LEU:H     | 1:135:A:GLY:H   | 18       | 0.16          |
| (1,305)  | 1:29:A:MET:H     | 1:42:A:VAL:H    | 11       | 0.16          |
| (1,305)  | 1:29:A:MET:H     | 1:42:A:VAL:H    | 13       | 0.16          |
| (1,305)  | 1:29:A:MET:H     | 1:42:A:VAL:H    | 19       | 0.16          |
| (1,305)  | 1:29:A:MET:H     | 1:42:A:VAL:H    | 20       | 0.16          |
| (1,291)  | 1:29:A:MET:HA    | 1:56:A:TRP:HE1  | 11       | 0.16          |
| (1,291)  | 1:29:A:MET:HA    | 1:56:A:TRP:HE1  | 13       | 0.16          |
| (1,242)  | 1:26:A:TYR:HA    | 1:46:A:LEU:H    | 1        | 0.16          |
| (1,225)  | 1:23:A:SER:H     | 1:25:A:GLY:H    | 8        | 0.16          |
| (1,210)  | 1:22:A:ASN:H     | 1:156:A:ASP:H   | 4        | 0.16          |
| (1,195)  | 1:21:A:ASN:H     | 1:155:A:TRP:HH2 | 17       | 0.16          |
| (1,115)  | 1:17:A:PHE:H     | 1:56:A:TRP:HA   | 11       | 0.16          |
| (1,98)   | 1:16:A:TRP:HD1   | 1:16:A:TRP:H    | 2        | 0.16          |
| (1,98)   | 1:16:A:TRP:HD1   | 1:16:A:TRP:H    | 11       | 0.16          |
| (1,98)   | 1:16:A:TRP:HD1   | 1:16:A:TRP:H    | 13       | 0.16          |
| (1,1639) | 1:115:A:LEU:HD11 | 1:118:A:LYS:HB2 | 7        | 0.15          |
| (1,1639) | 1:115:A:LEU:HD11 | 1:118:A:LYS:HB3 | 7        | 0.15          |
| (1,1639) | 1:115:A:LEU:HD12 | 1:118:A:LYS:HB2 | 7        | 0.15          |
| (1,1639) | 1:115:A:LEU:HD12 | 1:118:A:LYS:HB3 | 7        | 0.15          |
| (1,1639) | 1:115:A:LEU:HD13 | 1:118:A:LYS:HB2 | 7        | 0.15          |
| (1,1639) | 1:115:A:LEU:HD13 | 1:118:A:LYS:HB3 | 7        | 0.15          |
| (1,1639) | 1:115:A:LEU:HD21 | 1:118:A:LYS:HB2 | 7        | 0.15          |
| (1,1639) | 1:115:A:LEU:HD21 | 1:118:A:LYS:HB3 | 7        | 0.15          |
| (1,1639) | 1:115:A:LEU:HD22 | 1:118:A:LYS:HB2 | 7        | 0.15          |
| (1,1639) | 1:115:A:LEU:HD22 | 1:118:A:LYS:HB3 | 7        | 0.15          |
| (1,1639) | 1:115:A:LEU:HD23 | 1:118:A:LYS:HB2 | 7        | 0.15          |
| (1,1639) | 1:115:A:LEU:HD23 | 1:118:A:LYS:HB3 | 7        | 0.15          |
| (1,1542) | 1:162:A:VAL:HB   | 1:162:A:VAL:H   | 5        | 0.15          |
| (1,1542) | 1:162:A:VAL:HB   | 1:162:A:VAL:H   | 6        | 0.15          |
| (1,1485) | 1:152:A:GLU:H    | 1:154:A:ARG:H   | 4        | 0.15          |
| (1,1442) | 1:149:A:ASP:HA   | 1:150:A:ARG:H   | 17       | 0.15          |
| (1,1431) | 1:147:A:HIS:H    | 1:148:A:LEU:HG  | 18       | 0.15          |
| (1,1405) | 1:145:A:LYS:HA   | 1:147:A:HIS:H   | 6        | 0.15          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1364) | 1:139:A:HIS:HD2 | 1:139:A:HIS:H    | 2        | 0.15          |
| (1,1321) | 1:133:A:ARG:HA  | 1:136:A:LEU:H    | 10       | 0.15          |
| (1,1321) | 1:133:A:ARG:HA  | 1:136:A:LEU:H    | 13       | 0.15          |
| (1,1294) | 1:129:A:PHE:HA  | 1:131:A:ALA:H    | 1        | 0.15          |
| (1,1294) | 1:129:A:PHE:HA  | 1:131:A:ALA:H    | 4        | 0.15          |
| (1,1294) | 1:129:A:PHE:HA  | 1:131:A:ALA:H    | 12       | 0.15          |
| (1,1294) | 1:129:A:PHE:HA  | 1:131:A:ALA:H    | 16       | 0.15          |
| (1,1163) | 1:115:A:LEU:HG  | 1:120:A:SER:H    | 2        | 0.15          |
| (1,1160) | 1:115:A:LEU:HG  | 1:116:A:ALA:H    | 2        | 0.15          |
| (1,1160) | 1:115:A:LEU:HG  | 1:116:A:ALA:H    | 5        | 0.15          |
| (1,1160) | 1:115:A:LEU:HG  | 1:116:A:ALA:H    | 15       | 0.15          |
| (1,1155) | 1:115:A:LEU:HB2 | 1:118:A:LYS:H    | 7        | 0.15          |
| (1,1155) | 1:115:A:LEU:HB3 | 1:118:A:LYS:H    | 7        | 0.15          |
| (1,1145) | 1:114:A:TYR:HD1 | 1:115:A:LEU:H    | 20       | 0.15          |
| (1,1097) | 1:108:A:SER:H   | 1:114:A:TYR:HE1  | 2        | 0.15          |
| (1,1096) | 1:108:A:SER:H   | 1:112:A:HIS:H    | 5        | 0.15          |
| (1,1073) | 1:106:A:GLY:H   | 1:114:A:TYR:H    | 2        | 0.15          |
| (1,999)  | 1:98:A:ASP:HA   | 1:101:A:ASN:HD22 | 1        | 0.15          |
| (1,998)  | 1:98:A:ASP:HA   | 1:100:A:LEU:H    | 20       | 0.15          |
| (1,992)  | 1:97:A:LYS:HG2  | 1:97:A:LYS:H     | 2        | 0.15          |
| (1,992)  | 1:97:A:LYS:HG3  | 1:97:A:LYS:H     | 2        | 0.15          |
| (1,992)  | 1:97:A:LYS:HG2  | 1:97:A:LYS:H     | 4        | 0.15          |
| (1,992)  | 1:97:A:LYS:HG3  | 1:97:A:LYS:H     | 4        | 0.15          |
| (1,960)  | 1:95:A:ASN:HA   | 1:96:A:VAL:H     | 14       | 0.15          |
| (1,927)  | 1:90:A:THR:HB   | 1:91:A:GLN:H     | 16       | 0.15          |
| (1,881)  | 1:84:A:VAL:H    | 1:140:A:LEU:H    | 3        | 0.15          |
| (1,881)  | 1:84:A:VAL:H    | 1:140:A:LEU:H    | 6        | 0.15          |
| (1,881)  | 1:84:A:VAL:H    | 1:140:A:LEU:H    | 12       | 0.15          |
| (1,881)  | 1:84:A:VAL:H    | 1:140:A:LEU:H    | 14       | 0.15          |
| (1,864)  | 1:83:A:GLY:H    | 1:139:A:HIS:HD2  | 20       | 0.15          |
| (1,783)  | 1:75:A:ILE:HB   | 1:76:A:ALA:H     | 2        | 0.15          |
| (1,783)  | 1:75:A:ILE:HB   | 1:76:A:ALA:H     | 3        | 0.15          |
| (1,783)  | 1:75:A:ILE:HB   | 1:76:A:ALA:H     | 19       | 0.15          |
| (1,754)  | 1:72:A:VAL:H    | 1:89:A:GLN:H     | 5        | 0.15          |
| (1,695)  | 1:66:A:ASN:H    | 1:69:A:SER:H     | 15       | 0.15          |
| (1,623)  | 1:59:A:ASP:H    | 1:63:A:TYR:HD1   | 16       | 0.15          |
| (1,612)  | 1:58:A:HIS:HD2  | 1:59:A:ASP:H     | 16       | 0.15          |
| (1,570)  | 1:55:A:LEU:H    | 1:56:A:TRP:HE1   | 17       | 0.15          |
| (1,483)  | 1:46:A:LEU:HG   | 1:46:A:LEU:H     | 5        | 0.15          |
| (1,483)  | 1:46:A:LEU:HG   | 1:46:A:LEU:H     | 10       | 0.15          |
| (1,483)  | 1:46:A:LEU:HG   | 1:46:A:LEU:H     | 12       | 0.15          |
| (1,483)  | 1:46:A:LEU:HG   | 1:46:A:LEU:H     | 19       | 0.15          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,468)  | 1:45:A:THR:HB    | 1:46:A:LEU:H    | 13       | 0.15          |
| (1,453)  | 1:43:A:LEU:H     | 1:135:A:GLY:H   | 8        | 0.15          |
| (1,363)  | 1:34:A:SER:H     | 1:36:A:GLU:H    | 4        | 0.15          |
| (1,363)  | 1:34:A:SER:H     | 1:36:A:GLU:H    | 15       | 0.15          |
| (1,305)  | 1:29:A:MET:H     | 1:42:A:VAL:H    | 3        | 0.15          |
| (1,305)  | 1:29:A:MET:H     | 1:42:A:VAL:H    | 6        | 0.15          |
| (1,305)  | 1:29:A:MET:H     | 1:42:A:VAL:H    | 15       | 0.15          |
| (1,305)  | 1:29:A:MET:H     | 1:42:A:VAL:H    | 18       | 0.15          |
| (1,291)  | 1:29:A:MET:HA    | 1:56:A:TRP:HE1  | 18       | 0.15          |
| (1,291)  | 1:29:A:MET:HA    | 1:56:A:TRP:HE1  | 20       | 0.15          |
| (1,285)  | 1:28:A:LEU:HG    | 1:29:A:MET:H    | 12       | 0.15          |
| (1,285)  | 1:28:A:LEU:HG    | 1:29:A:MET:H    | 19       | 0.15          |
| (1,225)  | 1:23:A:SER:H     | 1:25:A:GLY:H    | 3        | 0.15          |
| (1,223)  | 1:23:A:SER:H     | 1:152:A:GLU:H   | 11       | 0.15          |
| (1,223)  | 1:23:A:SER:H     | 1:152:A:GLU:H   | 20       | 0.15          |
| (1,210)  | 1:22:A:ASN:H     | 1:156:A:ASP:H   | 3        | 0.15          |
| (1,210)  | 1:22:A:ASN:H     | 1:156:A:ASP:H   | 16       | 0.15          |
| (1,195)  | 1:21:A:ASN:H     | 1:155:A:TRP:HH2 | 1        | 0.15          |
| (1,115)  | 1:17:A:PHE:H     | 1:56:A:TRP:HA   | 1        | 0.15          |
| (1,115)  | 1:17:A:PHE:H     | 1:56:A:TRP:HA   | 7        | 0.15          |
| (1,115)  | 1:17:A:PHE:H     | 1:56:A:TRP:HA   | 12       | 0.15          |
| (1,115)  | 1:17:A:PHE:H     | 1:56:A:TRP:HA   | 14       | 0.15          |
| (1,98)   | 1:16:A:TRP:HD1   | 1:16:A:TRP:H    | 7        | 0.15          |
| (1,98)   | 1:16:A:TRP:HD1   | 1:16:A:TRP:H    | 8        | 0.15          |
| (1,98)   | 1:16:A:TRP:HD1   | 1:16:A:TRP:H    | 10       | 0.15          |
| (1,98)   | 1:16:A:TRP:HD1   | 1:16:A:TRP:H    | 12       | 0.15          |
| (1,98)   | 1:16:A:TRP:HD1   | 1:16:A:TRP:H    | 16       | 0.15          |
| (1,1639) | 1:115:A:LEU:HD11 | 1:118:A:LYS:HB2 | 9        | 0.14          |
| (1,1639) | 1:115:A:LEU:HD11 | 1:118:A:LYS:HB3 | 9        | 0.14          |
| (1,1639) | 1:115:A:LEU:HD12 | 1:118:A:LYS:HB2 | 9        | 0.14          |
| (1,1639) | 1:115:A:LEU:HD12 | 1:118:A:LYS:HB3 | 9        | 0.14          |
| (1,1639) | 1:115:A:LEU:HD13 | 1:118:A:LYS:HB2 | 9        | 0.14          |
| (1,1639) | 1:115:A:LEU:HD13 | 1:118:A:LYS:HB3 | 9        | 0.14          |
| (1,1639) | 1:115:A:LEU:HD21 | 1:118:A:LYS:HB2 | 9        | 0.14          |
| (1,1639) | 1:115:A:LEU:HD21 | 1:118:A:LYS:HB3 | 9        | 0.14          |
| (1,1639) | 1:115:A:LEU:HD22 | 1:118:A:LYS:HB2 | 9        | 0.14          |
| (1,1639) | 1:115:A:LEU:HD22 | 1:118:A:LYS:HB3 | 9        | 0.14          |
| (1,1639) | 1:115:A:LEU:HD23 | 1:118:A:LYS:HB2 | 9        | 0.14          |
| (1,1639) | 1:115:A:LEU:HD23 | 1:118:A:LYS:HB3 | 9        | 0.14          |
| (1,1639) | 1:115:A:LEU:HD11 | 1:118:A:LYS:HB2 | 20       | 0.14          |
| (1,1639) | 1:115:A:LEU:HD11 | 1:118:A:LYS:HB3 | 20       | 0.14          |
| (1,1639) | 1:115:A:LEU:HD12 | 1:118:A:LYS:HB2 | 20       | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1639) | 1:115:A:LEU:HD12 | 1:118:A:LYS:HB3  | 20       | 0.14          |
| (1,1639) | 1:115:A:LEU:HD13 | 1:118:A:LYS:HB2  | 20       | 0.14          |
| (1,1639) | 1:115:A:LEU:HD13 | 1:118:A:LYS:HB3  | 20       | 0.14          |
| (1,1639) | 1:115:A:LEU:HD21 | 1:118:A:LYS:HB2  | 20       | 0.14          |
| (1,1639) | 1:115:A:LEU:HD21 | 1:118:A:LYS:HB3  | 20       | 0.14          |
| (1,1639) | 1:115:A:LEU:HD22 | 1:118:A:LYS:HB2  | 20       | 0.14          |
| (1,1639) | 1:115:A:LEU:HD22 | 1:118:A:LYS:HB3  | 20       | 0.14          |
| (1,1639) | 1:115:A:LEU:HD23 | 1:118:A:LYS:HB2  | 20       | 0.14          |
| (1,1639) | 1:115:A:LEU:HD23 | 1:118:A:LYS:HB3  | 20       | 0.14          |
| (1,1461) | 1:150:A:ARG:H    | 1:152:A:GLU:H    | 10       | 0.14          |
| (1,1431) | 1:147:A:HIS:H    | 1:148:A:LEU:HG   | 13       | 0.14          |
| (1,1431) | 1:147:A:HIS:H    | 1:148:A:LEU:HG   | 14       | 0.14          |
| (1,1431) | 1:147:A:HIS:H    | 1:148:A:LEU:HG   | 19       | 0.14          |
| (1,1321) | 1:133:A:ARG:HA   | 1:136:A:LEU:H    | 14       | 0.14          |
| (1,1310) | 1:132:A:ARG:HA   | 1:134:A:GLU:H    | 14       | 0.14          |
| (1,1241) | 1:123:A:LEU:HG   | 1:123:A:LEU:H    | 13       | 0.14          |
| (1,1160) | 1:115:A:LEU:HG   | 1:116:A:ALA:H    | 4        | 0.14          |
| (1,1160) | 1:115:A:LEU:HG   | 1:116:A:ALA:H    | 6        | 0.14          |
| (1,1160) | 1:115:A:LEU:HG   | 1:116:A:ALA:H    | 19       | 0.14          |
| (1,1155) | 1:115:A:LEU:HB2  | 1:118:A:LYS:H    | 10       | 0.14          |
| (1,1155) | 1:115:A:LEU:HB3  | 1:118:A:LYS:H    | 10       | 0.14          |
| (1,1145) | 1:114:A:TYR:HD1  | 1:115:A:LEU:H    | 15       | 0.14          |
| (1,1145) | 1:114:A:TYR:HD1  | 1:115:A:LEU:H    | 17       | 0.14          |
| (1,999)  | 1:98:A:ASP:HA    | 1:101:A:ASN:HD22 | 14       | 0.14          |
| (1,998)  | 1:98:A:ASP:HA    | 1:100:A:LEU:H    | 1        | 0.14          |
| (1,992)  | 1:97:A:LYS:HG2   | 1:97:A:LYS:H     | 1        | 0.14          |
| (1,992)  | 1:97:A:LYS:HG3   | 1:97:A:LYS:H     | 1        | 0.14          |
| (1,992)  | 1:97:A:LYS:HG2   | 1:97:A:LYS:H     | 3        | 0.14          |
| (1,992)  | 1:97:A:LYS:HG3   | 1:97:A:LYS:H     | 3        | 0.14          |
| (1,992)  | 1:97:A:LYS:HG2   | 1:97:A:LYS:H     | 6        | 0.14          |
| (1,992)  | 1:97:A:LYS:HG3   | 1:97:A:LYS:H     | 6        | 0.14          |
| (1,992)  | 1:97:A:LYS:HG2   | 1:97:A:LYS:H     | 8        | 0.14          |
| (1,992)  | 1:97:A:LYS:HG3   | 1:97:A:LYS:H     | 8        | 0.14          |
| (1,992)  | 1:97:A:LYS:HG2   | 1:97:A:LYS:H     | 12       | 0.14          |
| (1,992)  | 1:97:A:LYS:HG3   | 1:97:A:LYS:H     | 12       | 0.14          |
| (1,992)  | 1:97:A:LYS:HG2   | 1:97:A:LYS:H     | 14       | 0.14          |
| (1,992)  | 1:97:A:LYS:HG3   | 1:97:A:LYS:H     | 14       | 0.14          |
| (1,960)  | 1:95:A:ASN:HA    | 1:96:A:VAL:H     | 5        | 0.14          |
| (1,927)  | 1:90:A:THR:HB    | 1:91:A:GLN:H     | 1        | 0.14          |
| (1,927)  | 1:90:A:THR:HB    | 1:91:A:GLN:H     | 7        | 0.14          |
| (1,881)  | 1:84:A:VAL:H     | 1:140:A:LEU:H    | 1        | 0.14          |
| (1,881)  | 1:84:A:VAL:H     | 1:140:A:LEU:H    | 7        | 0.14          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,881) | 1:84:A:VAL:H   | 1:140:A:LEU:H   | 18       | 0.14          |
| (1,864) | 1:83:A:GLY:H   | 1:139:A:HIS:HD2 | 16       | 0.14          |
| (1,864) | 1:83:A:GLY:H   | 1:139:A:HIS:HD2 | 19       | 0.14          |
| (1,783) | 1:75:A:ILE:HB  | 1:76:A:ALA:H    | 15       | 0.14          |
| (1,754) | 1:72:A:VAL:H   | 1:89:A:GLN:H    | 11       | 0.14          |
| (1,728) | 1:69:A:SER:H   | 1:71:A:GLN:H    | 4        | 0.14          |
| (1,728) | 1:69:A:SER:H   | 1:71:A:GLN:H    | 9        | 0.14          |
| (1,711) | 1:68:A:LYS:HA  | 1:69:A:SER:H    | 20       | 0.14          |
| (1,659) | 1:63:A:TYR:HE1 | 1:92:A:ALA:H    | 11       | 0.14          |
| (1,659) | 1:63:A:TYR:HE2 | 1:92:A:ALA:H    | 11       | 0.14          |
| (1,647) | 1:62:A:GLY:H   | 1:63:A:TYR:HD1  | 4        | 0.14          |
| (1,629) | 1:60:A:PRO:HA  | 1:62:A:GLY:H    | 5        | 0.14          |
| (1,629) | 1:60:A:PRO:HA  | 1:62:A:GLY:H    | 8        | 0.14          |
| (1,623) | 1:59:A:ASP:H   | 1:63:A:TYR:HD1  | 5        | 0.14          |
| (1,623) | 1:59:A:ASP:H   | 1:63:A:TYR:HD1  | 19       | 0.14          |
| (1,603) | 1:57:A:ARG:H   | 1:65:A:VAL:HB   | 3        | 0.14          |
| (1,603) | 1:57:A:ARG:H   | 1:65:A:VAL:HB   | 12       | 0.14          |
| (1,570) | 1:55:A:LEU:H   | 1:56:A:TRP:HE1  | 2        | 0.14          |
| (1,570) | 1:55:A:LEU:H   | 1:56:A:TRP:HE1  | 15       | 0.14          |
| (1,570) | 1:55:A:LEU:H   | 1:56:A:TRP:HE1  | 18       | 0.14          |
| (1,545) | 1:53:A:SER:HA  | 1:68:A:LYS:H    | 3        | 0.14          |
| (1,483) | 1:46:A:LEU:HG  | 1:46:A:LEU:H    | 2        | 0.14          |
| (1,483) | 1:46:A:LEU:HG  | 1:46:A:LEU:H    | 4        | 0.14          |
| (1,483) | 1:46:A:LEU:HG  | 1:46:A:LEU:H    | 8        | 0.14          |
| (1,468) | 1:45:A:THR:HB  | 1:46:A:LEU:H    | 4        | 0.14          |
| (1,468) | 1:45:A:THR:HB  | 1:46:A:LEU:H    | 6        | 0.14          |
| (1,468) | 1:45:A:THR:HB  | 1:46:A:LEU:H    | 19       | 0.14          |
| (1,453) | 1:43:A:LEU:H   | 1:135:A:GLY:H   | 6        | 0.14          |
| (1,453) | 1:43:A:LEU:H   | 1:135:A:GLY:H   | 13       | 0.14          |
| (1,453) | 1:43:A:LEU:H   | 1:135:A:GLY:H   | 20       | 0.14          |
| (1,334) | 1:31:A:ASP:H   | 1:41:A:ILE:HA   | 1        | 0.14          |
| (1,305) | 1:29:A:MET:H   | 1:42:A:VAL:H    | 4        | 0.14          |
| (1,305) | 1:29:A:MET:H   | 1:42:A:VAL:H    | 7        | 0.14          |
| (1,305) | 1:29:A:MET:H   | 1:42:A:VAL:H    | 14       | 0.14          |
| (1,291) | 1:29:A:MET:HA  | 1:56:A:TRP:HE1  | 6        | 0.14          |
| (1,286) | 1:28:A:LEU:HG  | 1:56:A:TRP:HE1  | 2        | 0.14          |
| (1,286) | 1:28:A:LEU:HG  | 1:56:A:TRP:HE1  | 15       | 0.14          |
| (1,286) | 1:28:A:LEU:HG  | 1:56:A:TRP:HE1  | 18       | 0.14          |
| (1,285) | 1:28:A:LEU:HG  | 1:29:A:MET:H    | 14       | 0.14          |
| (1,242) | 1:26:A:TYR:HA  | 1:46:A:LEU:H    | 10       | 0.14          |
| (1,242) | 1:26:A:TYR:HA  | 1:46:A:LEU:H    | 16       | 0.14          |
| (1,242) | 1:26:A:TYR:HA  | 1:46:A:LEU:H    | 18       | 0.14          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,225)  | 1:23:A:SER:H     | 1:25:A:GLY:H    | 6        | 0.14          |
| (1,223)  | 1:23:A:SER:H     | 1:152:A:GLU:H   | 7        | 0.14          |
| (1,212)  | 1:23:A:SER:HA    | 1:152:A:GLU:H   | 10       | 0.14          |
| (1,210)  | 1:22:A:ASN:H     | 1:156:A:ASP:H   | 14       | 0.14          |
| (1,115)  | 1:17:A:PHE:H     | 1:56:A:TRP:HA   | 4        | 0.14          |
| (1,115)  | 1:17:A:PHE:H     | 1:56:A:TRP:HA   | 6        | 0.14          |
| (1,115)  | 1:17:A:PHE:H     | 1:56:A:TRP:HA   | 13       | 0.14          |
| (1,115)  | 1:17:A:PHE:H     | 1:56:A:TRP:HA   | 17       | 0.14          |
| (1,98)   | 1:16:A:TRP:HD1   | 1:16:A:TRP:H    | 17       | 0.14          |
| (1,45)   | 1:9:A:SER:HA     | 1:107:A:LEU:H   | 14       | 0.14          |
| (1,29)   | 1:6:A:PHE:H      | 1:7:A:GLU:H     | 11       | 0.14          |
| (1,1639) | 1:115:A:LEU:HD11 | 1:118:A:LYS:HB2 | 1        | 0.13          |
| (1,1639) | 1:115:A:LEU:HD11 | 1:118:A:LYS:HB3 | 1        | 0.13          |
| (1,1639) | 1:115:A:LEU:HD12 | 1:118:A:LYS:HB2 | 1        | 0.13          |
| (1,1639) | 1:115:A:LEU:HD12 | 1:118:A:LYS:HB3 | 1        | 0.13          |
| (1,1639) | 1:115:A:LEU:HD13 | 1:118:A:LYS:HB2 | 1        | 0.13          |
| (1,1639) | 1:115:A:LEU:HD13 | 1:118:A:LYS:HB3 | 1        | 0.13          |
| (1,1639) | 1:115:A:LEU:HD21 | 1:118:A:LYS:HB2 | 1        | 0.13          |
| (1,1639) | 1:115:A:LEU:HD21 | 1:118:A:LYS:HB3 | 1        | 0.13          |
| (1,1639) | 1:115:A:LEU:HD22 | 1:118:A:LYS:HB2 | 1        | 0.13          |
| (1,1639) | 1:115:A:LEU:HD22 | 1:118:A:LYS:HB3 | 1        | 0.13          |
| (1,1639) | 1:115:A:LEU:HD23 | 1:118:A:LYS:HB2 | 1        | 0.13          |
| (1,1639) | 1:115:A:LEU:HD23 | 1:118:A:LYS:HB3 | 1        | 0.13          |
| (1,1639) | 1:115:A:LEU:HD11 | 1:118:A:LYS:HB2 | 15       | 0.13          |
| (1,1639) | 1:115:A:LEU:HD11 | 1:118:A:LYS:HB3 | 15       | 0.13          |
| (1,1639) | 1:115:A:LEU:HD12 | 1:118:A:LYS:HB2 | 15       | 0.13          |
| (1,1639) | 1:115:A:LEU:HD12 | 1:118:A:LYS:HB3 | 15       | 0.13          |
| (1,1639) | 1:115:A:LEU:HD13 | 1:118:A:LYS:HB2 | 15       | 0.13          |
| (1,1639) | 1:115:A:LEU:HD13 | 1:118:A:LYS:HB3 | 15       | 0.13          |
| (1,1639) | 1:115:A:LEU:HD21 | 1:118:A:LYS:HB2 | 15       | 0.13          |
| (1,1639) | 1:115:A:LEU:HD21 | 1:118:A:LYS:HB3 | 15       | 0.13          |
| (1,1639) | 1:115:A:LEU:HD22 | 1:118:A:LYS:HB2 | 15       | 0.13          |
| (1,1639) | 1:115:A:LEU:HD22 | 1:118:A:LYS:HB3 | 15       | 0.13          |
| (1,1639) | 1:115:A:LEU:HD23 | 1:118:A:LYS:HB2 | 15       | 0.13          |
| (1,1639) | 1:115:A:LEU:HD23 | 1:118:A:LYS:HB3 | 15       | 0.13          |
| (1,1479) | 1:152:A:GLU:HA   | 1:154:A:ARG:H   | 3        | 0.13          |
| (1,1461) | 1:150:A:ARG:H    | 1:152:A:GLU:H   | 9        | 0.13          |
| (1,1449) | 1:150:A:ARG:HA   | 1:152:A:GLU:H   | 9        | 0.13          |
| (1,1442) | 1:149:A:ASP:HA   | 1:150:A:ARG:H   | 14       | 0.13          |
| (1,1431) | 1:147:A:HIS:H    | 1:148:A:LEU:HG  | 1        | 0.13          |
| (1,1431) | 1:147:A:HIS:H    | 1:148:A:LEU:HG  | 7        | 0.13          |
| (1,1321) | 1:133:A:ARG:HA   | 1:136:A:LEU:H   | 6        | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1283) | 1:127:A:GLU:HG2 | 1:127:A:GLU:H   | 20       | 0.13          |
| (1,1283) | 1:127:A:GLU:HG3 | 1:127:A:GLU:H   | 20       | 0.13          |
| (1,1160) | 1:115:A:LEU:HG  | 1:116:A:ALA:H   | 10       | 0.13          |
| (1,1160) | 1:115:A:LEU:HG  | 1:116:A:ALA:H   | 12       | 0.13          |
| (1,1160) | 1:115:A:LEU:HG  | 1:116:A:ALA:H   | 17       | 0.13          |
| (1,1155) | 1:115:A:LEU:HB2 | 1:118:A:LYS:H   | 9        | 0.13          |
| (1,1155) | 1:115:A:LEU:HB3 | 1:118:A:LYS:H   | 9        | 0.13          |
| (1,1145) | 1:114:A:TYR:HD1 | 1:115:A:LEU:H   | 3        | 0.13          |
| (1,1097) | 1:108:A:SER:H   | 1:114:A:TYR:HE1 | 4        | 0.13          |
| (1,1097) | 1:108:A:SER:H   | 1:114:A:TYR:HE1 | 9        | 0.13          |
| (1,1097) | 1:108:A:SER:H   | 1:114:A:TYR:HE1 | 10       | 0.13          |
| (1,1097) | 1:108:A:SER:H   | 1:114:A:TYR:HE1 | 19       | 0.13          |
| (1,1096) | 1:108:A:SER:H   | 1:112:A:HIS:H   | 17       | 0.13          |
| (1,1016) | 1:99:A:ASP:H    | 1:101:A:ASN:H   | 20       | 0.13          |
| (1,992)  | 1:97:A:LYS:HG2  | 1:97:A:LYS:H    | 5        | 0.13          |
| (1,992)  | 1:97:A:LYS:HG3  | 1:97:A:LYS:H    | 5        | 0.13          |
| (1,992)  | 1:97:A:LYS:HG2  | 1:97:A:LYS:H    | 7        | 0.13          |
| (1,992)  | 1:97:A:LYS:HG3  | 1:97:A:LYS:H    | 7        | 0.13          |
| (1,992)  | 1:97:A:LYS:HG2  | 1:97:A:LYS:H    | 10       | 0.13          |
| (1,992)  | 1:97:A:LYS:HG3  | 1:97:A:LYS:H    | 10       | 0.13          |
| (1,992)  | 1:97:A:LYS:HG2  | 1:97:A:LYS:H    | 13       | 0.13          |
| (1,992)  | 1:97:A:LYS:HG3  | 1:97:A:LYS:H    | 13       | 0.13          |
| (1,992)  | 1:97:A:LYS:HG2  | 1:97:A:LYS:H    | 15       | 0.13          |
| (1,992)  | 1:97:A:LYS:HG3  | 1:97:A:LYS:H    | 15       | 0.13          |
| (1,992)  | 1:97:A:LYS:HG2  | 1:97:A:LYS:H    | 17       | 0.13          |
| (1,992)  | 1:97:A:LYS:HG3  | 1:97:A:LYS:H    | 17       | 0.13          |
| (1,992)  | 1:97:A:LYS:HG2  | 1:97:A:LYS:H    | 18       | 0.13          |
| (1,992)  | 1:97:A:LYS:HG3  | 1:97:A:LYS:H    | 18       | 0.13          |
| (1,992)  | 1:97:A:LYS:HG2  | 1:97:A:LYS:H    | 19       | 0.13          |
| (1,992)  | 1:97:A:LYS:HG3  | 1:97:A:LYS:H    | 19       | 0.13          |
| (1,927)  | 1:90:A:THR:HB   | 1:91:A:GLN:H    | 20       | 0.13          |
| (1,881)  | 1:84:A:VAL:H    | 1:140:A:LEU:H   | 9        | 0.13          |
| (1,864)  | 1:83:A:GLY:H    | 1:139:A:HIS:HD2 | 6        | 0.13          |
| (1,711)  | 1:68:A:LYS:HA   | 1:69:A:SER:H    | 5        | 0.13          |
| (1,695)  | 1:66:A:ASN:H    | 1:69:A:SER:H    | 16       | 0.13          |
| (1,669)  | 1:64:A:LEU:HG   | 1:65:A:VAL:H    | 15       | 0.13          |
| (1,647)  | 1:62:A:GLY:H    | 1:63:A:TYR:HD1  | 5        | 0.13          |
| (1,647)  | 1:62:A:GLY:H    | 1:63:A:TYR:HD1  | 11       | 0.13          |
| (1,647)  | 1:62:A:GLY:H    | 1:63:A:TYR:HD1  | 13       | 0.13          |
| (1,629)  | 1:60:A:PRO:HA   | 1:62:A:GLY:H    | 20       | 0.13          |
| (1,623)  | 1:59:A:ASP:H    | 1:63:A:TYR:HD1  | 12       | 0.13          |
| (1,623)  | 1:59:A:ASP:H    | 1:63:A:TYR:HD1  | 14       | 0.13          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,488)  | 1:47:A:ARG:HA    | 1:49:A:LYS:H    | 10       | 0.13          |
| (1,483)  | 1:46:A:LEU:HG    | 1:46:A:LEU:H    | 9        | 0.13          |
| (1,483)  | 1:46:A:LEU:HG    | 1:46:A:LEU:H    | 11       | 0.13          |
| (1,483)  | 1:46:A:LEU:HG    | 1:46:A:LEU:H    | 13       | 0.13          |
| (1,483)  | 1:46:A:LEU:HG    | 1:46:A:LEU:H    | 16       | 0.13          |
| (1,483)  | 1:46:A:LEU:HG    | 1:46:A:LEU:H    | 20       | 0.13          |
| (1,468)  | 1:45:A:THR:HB    | 1:46:A:LEU:H    | 11       | 0.13          |
| (1,468)  | 1:45:A:THR:HB    | 1:46:A:LEU:H    | 20       | 0.13          |
| (1,330)  | 1:31:A:ASP:HA    | 1:32:A:ASN:H    | 1        | 0.13          |
| (1,330)  | 1:31:A:ASP:HA    | 1:32:A:ASN:H    | 9        | 0.13          |
| (1,291)  | 1:29:A:MET:HA    | 1:56:A:TRP:HE1  | 2        | 0.13          |
| (1,225)  | 1:23:A:SER:H     | 1:25:A:GLY:H    | 15       | 0.13          |
| (1,223)  | 1:23:A:SER:H     | 1:152:A:GLU:H   | 4        | 0.13          |
| (1,223)  | 1:23:A:SER:H     | 1:152:A:GLU:H   | 8        | 0.13          |
| (1,214)  | 1:23:A:SER:HA    | 1:24:A:ASN:H    | 15       | 0.13          |
| (1,212)  | 1:23:A:SER:HA    | 1:152:A:GLU:H   | 13       | 0.13          |
| (1,210)  | 1:22:A:ASN:H     | 1:156:A:ASP:H   | 18       | 0.13          |
| (1,210)  | 1:22:A:ASN:H     | 1:156:A:ASP:H   | 20       | 0.13          |
| (1,195)  | 1:21:A:ASN:H     | 1:155:A:TRP:HH2 | 3        | 0.13          |
| (1,195)  | 1:21:A:ASN:H     | 1:155:A:TRP:HH2 | 8        | 0.13          |
| (1,45)   | 1:9:A:SER:HA     | 1:107:A:LEU:H   | 12       | 0.13          |
| (1,1639) | 1:115:A:LEU:HD11 | 1:118:A:LYS:HB2 | 8        | 0.12          |
| (1,1639) | 1:115:A:LEU:HD11 | 1:118:A:LYS:HB3 | 8        | 0.12          |
| (1,1639) | 1:115:A:LEU:HD12 | 1:118:A:LYS:HB2 | 8        | 0.12          |
| (1,1639) | 1:115:A:LEU:HD12 | 1:118:A:LYS:HB3 | 8        | 0.12          |
| (1,1639) | 1:115:A:LEU:HD13 | 1:118:A:LYS:HB2 | 8        | 0.12          |
| (1,1639) | 1:115:A:LEU:HD13 | 1:118:A:LYS:HB3 | 8        | 0.12          |
| (1,1639) | 1:115:A:LEU:HD21 | 1:118:A:LYS:HB2 | 8        | 0.12          |
| (1,1639) | 1:115:A:LEU:HD21 | 1:118:A:LYS:HB3 | 8        | 0.12          |
| (1,1639) | 1:115:A:LEU:HD22 | 1:118:A:LYS:HB2 | 8        | 0.12          |
| (1,1639) | 1:115:A:LEU:HD22 | 1:118:A:LYS:HB3 | 8        | 0.12          |
| (1,1639) | 1:115:A:LEU:HD23 | 1:118:A:LYS:HB2 | 8        | 0.12          |
| (1,1639) | 1:115:A:LEU:HD23 | 1:118:A:LYS:HB3 | 8        | 0.12          |
| (1,1639) | 1:115:A:LEU:HD11 | 1:118:A:LYS:HB2 | 13       | 0.12          |
| (1,1639) | 1:115:A:LEU:HD11 | 1:118:A:LYS:HB3 | 13       | 0.12          |
| (1,1639) | 1:115:A:LEU:HD12 | 1:118:A:LYS:HB2 | 13       | 0.12          |
| (1,1639) | 1:115:A:LEU:HD12 | 1:118:A:LYS:HB3 | 13       | 0.12          |
| (1,1639) | 1:115:A:LEU:HD13 | 1:118:A:LYS:HB2 | 13       | 0.12          |
| (1,1639) | 1:115:A:LEU:HD13 | 1:118:A:LYS:HB3 | 13       | 0.12          |
| (1,1639) | 1:115:A:LEU:HD21 | 1:118:A:LYS:HB2 | 13       | 0.12          |
| (1,1639) | 1:115:A:LEU:HD21 | 1:118:A:LYS:HB3 | 13       | 0.12          |
| (1,1639) | 1:115:A:LEU:HD22 | 1:118:A:LYS:HB2 | 13       | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1639) | 1:115:A:LEU:HD22 | 1:118:A:LYS:HB3  | 13       | 0.12          |
| (1,1639) | 1:115:A:LEU:HD23 | 1:118:A:LYS:HB2  | 13       | 0.12          |
| (1,1639) | 1:115:A:LEU:HD23 | 1:118:A:LYS:HB3  | 13       | 0.12          |
| (1,1479) | 1:152:A:GLU:HA   | 1:154:A:ARG:H    | 10       | 0.12          |
| (1,1431) | 1:147:A:HIS:H    | 1:148:A:LEU:HG   | 6        | 0.12          |
| (1,1431) | 1:147:A:HIS:H    | 1:148:A:LEU:HG   | 8        | 0.12          |
| (1,1431) | 1:147:A:HIS:H    | 1:148:A:LEU:HG   | 9        | 0.12          |
| (1,1431) | 1:147:A:HIS:H    | 1:148:A:LEU:HG   | 11       | 0.12          |
| (1,1431) | 1:147:A:HIS:H    | 1:148:A:LEU:HG   | 15       | 0.12          |
| (1,1405) | 1:145:A:LYS:HA   | 1:147:A:HIS:H    | 9        | 0.12          |
| (1,1405) | 1:145:A:LYS:HA   | 1:147:A:HIS:H    | 16       | 0.12          |
| (1,1405) | 1:145:A:LYS:HA   | 1:147:A:HIS:H    | 18       | 0.12          |
| (1,1364) | 1:139:A:HIS:HD2  | 1:139:A:HIS:H    | 6        | 0.12          |
| (1,1338) | 1:135:A:GLY:H    | 1:136:A:LEU:H    | 3        | 0.12          |
| (1,1318) | 1:132:A:ARG:HG2  | 1:134:A:GLU:H    | 2        | 0.12          |
| (1,1318) | 1:132:A:ARG:HG3  | 1:134:A:GLU:H    | 2        | 0.12          |
| (1,1310) | 1:132:A:ARG:HA   | 1:134:A:GLU:H    | 5        | 0.12          |
| (1,1294) | 1:129:A:PHE:HA   | 1:131:A:ALA:H    | 2        | 0.12          |
| (1,1160) | 1:115:A:LEU:HG   | 1:116:A:ALA:H    | 3        | 0.12          |
| (1,1160) | 1:115:A:LEU:HG   | 1:116:A:ALA:H    | 9        | 0.12          |
| (1,1160) | 1:115:A:LEU:HG   | 1:116:A:ALA:H    | 11       | 0.12          |
| (1,1160) | 1:115:A:LEU:HG   | 1:116:A:ALA:H    | 14       | 0.12          |
| (1,1160) | 1:115:A:LEU:HG   | 1:116:A:ALA:H    | 18       | 0.12          |
| (1,1160) | 1:115:A:LEU:HG   | 1:116:A:ALA:H    | 20       | 0.12          |
| (1,1145) | 1:114:A:TYR:HD1  | 1:115:A:LEU:H    | 1        | 0.12          |
| (1,1145) | 1:114:A:TYR:HD1  | 1:115:A:LEU:H    | 7        | 0.12          |
| (1,1097) | 1:108:A:SER:H    | 1:114:A:TYR:HE1  | 5        | 0.12          |
| (1,1097) | 1:108:A:SER:H    | 1:114:A:TYR:HE1  | 6        | 0.12          |
| (1,1080) | 1:107:A:LEU:HA   | 1:114:A:TYR:H    | 20       | 0.12          |
| (1,999)  | 1:98:A:ASP:HA    | 1:101:A:ASN:HD22 | 20       | 0.12          |
| (1,998)  | 1:98:A:ASP:HA    | 1:100:A:LEU:H    | 16       | 0.12          |
| (1,955)  | 1:94:A:SER:HA    | 1:95:A:ASN:H     | 18       | 0.12          |
| (1,952)  | 1:93:A:GLY:H     | 1:96:A:VAL:HG11  | 18       | 0.12          |
| (1,952)  | 1:93:A:GLY:H     | 1:96:A:VAL:HG12  | 18       | 0.12          |
| (1,952)  | 1:93:A:GLY:H     | 1:96:A:VAL:HG13  | 18       | 0.12          |
| (1,952)  | 1:93:A:GLY:H     | 1:96:A:VAL:HG21  | 18       | 0.12          |
| (1,952)  | 1:93:A:GLY:H     | 1:96:A:VAL:HG22  | 18       | 0.12          |
| (1,952)  | 1:93:A:GLY:H     | 1:96:A:VAL:HG23  | 18       | 0.12          |
| (1,881)  | 1:84:A:VAL:H     | 1:140:A:LEU:H    | 20       | 0.12          |
| (1,864)  | 1:83:A:GLY:H     | 1:139:A:HIS:HD2  | 2        | 0.12          |
| (1,864)  | 1:83:A:GLY:H     | 1:139:A:HIS:HD2  | 5        | 0.12          |
| (1,783)  | 1:75:A:ILE:HB    | 1:76:A:ALA:H     | 4        | 0.12          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,728) | 1:69:A:SER:H  | 1:71:A:GLN:H   | 5        | 0.12          |
| (1,711) | 1:68:A:LYS:HA | 1:69:A:SER:H   | 1        | 0.12          |
| (1,711) | 1:68:A:LYS:HA | 1:69:A:SER:H   | 2        | 0.12          |
| (1,711) | 1:68:A:LYS:HA | 1:69:A:SER:H   | 3        | 0.12          |
| (1,711) | 1:68:A:LYS:HA | 1:69:A:SER:H   | 4        | 0.12          |
| (1,711) | 1:68:A:LYS:HA | 1:69:A:SER:H   | 6        | 0.12          |
| (1,711) | 1:68:A:LYS:HA | 1:69:A:SER:H   | 11       | 0.12          |
| (1,711) | 1:68:A:LYS:HA | 1:69:A:SER:H   | 12       | 0.12          |
| (1,711) | 1:68:A:LYS:HA | 1:69:A:SER:H   | 16       | 0.12          |
| (1,711) | 1:68:A:LYS:HA | 1:69:A:SER:H   | 17       | 0.12          |
| (1,695) | 1:66:A:ASN:H  | 1:69:A:SER:H   | 12       | 0.12          |
| (1,647) | 1:62:A:GLY:H  | 1:63:A:TYR:HD1 | 1        | 0.12          |
| (1,647) | 1:62:A:GLY:H  | 1:63:A:TYR:HD1 | 20       | 0.12          |
| (1,629) | 1:60:A:PRO:HA | 1:62:A:GLY:H   | 18       | 0.12          |
| (1,608) | 1:58:A:HIS:HA | 1:65:A:VAL:H   | 19       | 0.12          |
| (1,570) | 1:55:A:LEU:H  | 1:56:A:TRP:HE1 | 12       | 0.12          |
| (1,570) | 1:55:A:LEU:H  | 1:56:A:TRP:HE1 | 16       | 0.12          |
| (1,570) | 1:55:A:LEU:H  | 1:56:A:TRP:HE1 | 19       | 0.12          |
| (1,545) | 1:53:A:SER:HA | 1:68:A:LYS:H   | 7        | 0.12          |
| (1,545) | 1:53:A:SER:HA | 1:68:A:LYS:H   | 19       | 0.12          |
| (1,488) | 1:47:A:ARG:HA | 1:49:A:LYS:H   | 6        | 0.12          |
| (1,488) | 1:47:A:ARG:HA | 1:49:A:LYS:H   | 12       | 0.12          |
| (1,488) | 1:47:A:ARG:HA | 1:49:A:LYS:H   | 13       | 0.12          |
| (1,488) | 1:47:A:ARG:HA | 1:49:A:LYS:H   | 19       | 0.12          |
| (1,483) | 1:46:A:LEU:HG | 1:46:A:LEU:H   | 1        | 0.12          |
| (1,483) | 1:46:A:LEU:HG | 1:46:A:LEU:H   | 3        | 0.12          |
| (1,483) | 1:46:A:LEU:HG | 1:46:A:LEU:H   | 6        | 0.12          |
| (1,483) | 1:46:A:LEU:HG | 1:46:A:LEU:H   | 17       | 0.12          |
| (1,483) | 1:46:A:LEU:HG | 1:46:A:LEU:H   | 18       | 0.12          |
| (1,453) | 1:43:A:LEU:H  | 1:135:A:GLY:H  | 1        | 0.12          |
| (1,453) | 1:43:A:LEU:H  | 1:135:A:GLY:H  | 15       | 0.12          |
| (1,330) | 1:31:A:ASP:HA | 1:32:A:ASN:H   | 10       | 0.12          |
| (1,305) | 1:29:A:MET:H  | 1:42:A:VAL:H   | 5        | 0.12          |
| (1,305) | 1:29:A:MET:H  | 1:42:A:VAL:H   | 12       | 0.12          |
| (1,291) | 1:29:A:MET:HA | 1:56:A:TRP:HE1 | 9        | 0.12          |
| (1,291) | 1:29:A:MET:HA | 1:56:A:TRP:HE1 | 14       | 0.12          |
| (1,286) | 1:28:A:LEU:HG | 1:56:A:TRP:HE1 | 19       | 0.12          |
| (1,242) | 1:26:A:TYR:HA | 1:46:A:LEU:H   | 2        | 0.12          |
| (1,242) | 1:26:A:TYR:HA | 1:46:A:LEU:H   | 12       | 0.12          |
| (1,225) | 1:23:A:SER:H  | 1:25:A:GLY:H   | 17       | 0.12          |
| (1,214) | 1:23:A:SER:HA | 1:24:A:ASN:H   | 3        | 0.12          |
| (1,214) | 1:23:A:SER:HA | 1:24:A:ASN:H   | 6        | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,214)  | 1:23:A:SER:HA    | 1:24:A:ASN:H     | 7        | 0.12          |
| (1,214)  | 1:23:A:SER:HA    | 1:24:A:ASN:H     | 8        | 0.12          |
| (1,214)  | 1:23:A:SER:HA    | 1:24:A:ASN:H     | 18       | 0.12          |
| (1,195)  | 1:21:A:ASN:H     | 1:155:A:TRP:HH2  | 16       | 0.12          |
| (1,182)  | 1:21:A:ASN:HA    | 1:156:A:ASP:H    | 9        | 0.12          |
| (1,130)  | 1:18:A:PHE:H     | 1:158:A:VAL:HB   | 11       | 0.12          |
| (1,115)  | 1:17:A:PHE:H     | 1:56:A:TRP:HA    | 8        | 0.12          |
| (1,98)   | 1:16:A:TRP:HD1   | 1:16:A:TRP:H     | 9        | 0.12          |
| (1,45)   | 1:9:A:SER:HA     | 1:107:A:LEU:H    | 2        | 0.12          |
| (1,45)   | 1:9:A:SER:HA     | 1:107:A:LEU:H    | 17       | 0.12          |
| (1,1639) | 1:115:A:LEU:HD11 | 1:118:A:LYS:HB2  | 14       | 0.11          |
| (1,1639) | 1:115:A:LEU:HD11 | 1:118:A:LYS:HB3  | 14       | 0.11          |
| (1,1639) | 1:115:A:LEU:HD12 | 1:118:A:LYS:HB2  | 14       | 0.11          |
| (1,1639) | 1:115:A:LEU:HD12 | 1:118:A:LYS:HB3  | 14       | 0.11          |
| (1,1639) | 1:115:A:LEU:HD13 | 1:118:A:LYS:HB2  | 14       | 0.11          |
| (1,1639) | 1:115:A:LEU:HD13 | 1:118:A:LYS:HB3  | 14       | 0.11          |
| (1,1639) | 1:115:A:LEU:HD21 | 1:118:A:LYS:HB2  | 14       | 0.11          |
| (1,1639) | 1:115:A:LEU:HD21 | 1:118:A:LYS:HB3  | 14       | 0.11          |
| (1,1639) | 1:115:A:LEU:HD22 | 1:118:A:LYS:HB2  | 14       | 0.11          |
| (1,1639) | 1:115:A:LEU:HD22 | 1:118:A:LYS:HB3  | 14       | 0.11          |
| (1,1639) | 1:115:A:LEU:HD23 | 1:118:A:LYS:HB2  | 14       | 0.11          |
| (1,1639) | 1:115:A:LEU:HD23 | 1:118:A:LYS:HB3  | 14       | 0.11          |
| (1,1639) | 1:115:A:LEU:HD11 | 1:118:A:LYS:HB2  | 16       | 0.11          |
| (1,1639) | 1:115:A:LEU:HD11 | 1:118:A:LYS:HB3  | 16       | 0.11          |
| (1,1639) | 1:115:A:LEU:HD12 | 1:118:A:LYS:HB2  | 16       | 0.11          |
| (1,1639) | 1:115:A:LEU:HD12 | 1:118:A:LYS:HB3  | 16       | 0.11          |
| (1,1639) | 1:115:A:LEU:HD13 | 1:118:A:LYS:HB2  | 16       | 0.11          |
| (1,1639) | 1:115:A:LEU:HD13 | 1:118:A:LYS:HB3  | 16       | 0.11          |
| (1,1639) | 1:115:A:LEU:HD21 | 1:118:A:LYS:HB2  | 16       | 0.11          |
| (1,1639) | 1:115:A:LEU:HD21 | 1:118:A:LYS:HB3  | 16       | 0.11          |
| (1,1639) | 1:115:A:LEU:HD22 | 1:118:A:LYS:HB2  | 16       | 0.11          |
| (1,1639) | 1:115:A:LEU:HD22 | 1:118:A:LYS:HB3  | 16       | 0.11          |
| (1,1639) | 1:115:A:LEU:HD23 | 1:118:A:LYS:HB2  | 16       | 0.11          |
| (1,1639) | 1:115:A:LEU:HD23 | 1:118:A:LYS:HB3  | 16       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD11  | 1:138:A:VAL:HG11 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD11  | 1:138:A:VAL:HG12 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD11  | 1:138:A:VAL:HG13 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD11  | 1:138:A:VAL:HG21 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD11  | 1:138:A:VAL:HG22 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD11  | 1:138:A:VAL:HG23 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD12  | 1:138:A:VAL:HG11 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD12  | 1:138:A:VAL:HG12 | 19       | 0.11          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1588) | 1:28:A:LEU:HD12 | 1:138:A:VAL:HG13 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD12 | 1:138:A:VAL:HG21 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD12 | 1:138:A:VAL:HG22 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD12 | 1:138:A:VAL:HG23 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD13 | 1:138:A:VAL:HG11 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD13 | 1:138:A:VAL:HG12 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD13 | 1:138:A:VAL:HG13 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD13 | 1:138:A:VAL:HG21 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD13 | 1:138:A:VAL:HG22 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD13 | 1:138:A:VAL:HG23 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD21 | 1:138:A:VAL:HG11 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD21 | 1:138:A:VAL:HG12 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD21 | 1:138:A:VAL:HG13 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD21 | 1:138:A:VAL:HG21 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD21 | 1:138:A:VAL:HG22 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD21 | 1:138:A:VAL:HG23 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD22 | 1:138:A:VAL:HG11 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD22 | 1:138:A:VAL:HG12 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD22 | 1:138:A:VAL:HG13 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD22 | 1:138:A:VAL:HG21 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD22 | 1:138:A:VAL:HG22 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD22 | 1:138:A:VAL:HG23 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD23 | 1:138:A:VAL:HG11 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD23 | 1:138:A:VAL:HG12 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD23 | 1:138:A:VAL:HG13 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD23 | 1:138:A:VAL:HG21 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD23 | 1:138:A:VAL:HG22 | 19       | 0.11          |
| (1,1588) | 1:28:A:LEU:HD23 | 1:138:A:VAL:HG23 | 19       | 0.11          |
| (1,1479) | 1:152:A:GLU:HA  | 1:154:A:ARG:H    | 6        | 0.11          |
| (1,1479) | 1:152:A:GLU:HA  | 1:154:A:ARG:H    | 7        | 0.11          |
| (1,1479) | 1:152:A:GLU:HA  | 1:154:A:ARG:H    | 14       | 0.11          |
| (1,1449) | 1:150:A:ARG:HA  | 1:152:A:GLU:H    | 1        | 0.11          |
| (1,1449) | 1:150:A:ARG:HA  | 1:152:A:GLU:H    | 4        | 0.11          |
| (1,1449) | 1:150:A:ARG:HA  | 1:152:A:GLU:H    | 10       | 0.11          |
| (1,1405) | 1:145:A:LYS:HA  | 1:147:A:HIS:H    | 13       | 0.11          |
| (1,1402) | 1:144:A:ASP:H   | 1:145:A:LYS:H    | 1        | 0.11          |
| (1,1333) | 1:134:A:GLU:HG2 | 1:134:A:GLU:H    | 12       | 0.11          |
| (1,1333) | 1:134:A:GLU:HG3 | 1:134:A:GLU:H    | 12       | 0.11          |
| (1,1321) | 1:133:A:ARG:HA  | 1:136:A:LEU:H    | 17       | 0.11          |
| (1,1293) | 1:129:A:PHE:HA  | 1:130:A:PHE:H    | 5        | 0.11          |
| (1,1291) | 1:128:A:SER:H   | 1:131:A:ALA:HB1  | 2        | 0.11          |
| (1,1291) | 1:128:A:SER:H   | 1:131:A:ALA:HB2  | 2        | 0.11          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1291) | 1:128:A:SER:H   | 1:131:A:ALA:HB3  | 2        | 0.11          |
| (1,1160) | 1:115:A:LEU:HG  | 1:116:A:ALA:H    | 7        | 0.11          |
| (1,1160) | 1:115:A:LEU:HG  | 1:116:A:ALA:H    | 8        | 0.11          |
| (1,1145) | 1:114:A:TYR:HD1 | 1:115:A:LEU:H    | 14       | 0.11          |
| (1,1116) | 1:112:A:HIS:HA  | 1:155:A:TRP:HE1  | 2        | 0.11          |
| (1,1080) | 1:107:A:LEU:HA  | 1:114:A:TYR:H    | 3        | 0.11          |
| (1,1080) | 1:107:A:LEU:HA  | 1:114:A:TYR:H    | 5        | 0.11          |
| (1,999)  | 1:98:A:ASP:HA   | 1:101:A:ASN:HD22 | 3        | 0.11          |
| (1,881)  | 1:84:A:VAL:H    | 1:140:A:LEU:H    | 4        | 0.11          |
| (1,881)  | 1:84:A:VAL:H    | 1:140:A:LEU:H    | 8        | 0.11          |
| (1,754)  | 1:72:A:VAL:H    | 1:89:A:GLN:H     | 1        | 0.11          |
| (1,711)  | 1:68:A:LYS:HA   | 1:69:A:SER:H     | 7        | 0.11          |
| (1,711)  | 1:68:A:LYS:HA   | 1:69:A:SER:H     | 8        | 0.11          |
| (1,711)  | 1:68:A:LYS:HA   | 1:69:A:SER:H     | 9        | 0.11          |
| (1,711)  | 1:68:A:LYS:HA   | 1:69:A:SER:H     | 10       | 0.11          |
| (1,711)  | 1:68:A:LYS:HA   | 1:69:A:SER:H     | 13       | 0.11          |
| (1,711)  | 1:68:A:LYS:HA   | 1:69:A:SER:H     | 14       | 0.11          |
| (1,711)  | 1:68:A:LYS:HA   | 1:69:A:SER:H     | 15       | 0.11          |
| (1,711)  | 1:68:A:LYS:HA   | 1:69:A:SER:H     | 18       | 0.11          |
| (1,711)  | 1:68:A:LYS:HA   | 1:69:A:SER:H     | 19       | 0.11          |
| (1,702)  | 1:67:A:LYS:HA   | 1:68:A:LYS:H     | 2        | 0.11          |
| (1,702)  | 1:67:A:LYS:HA   | 1:68:A:LYS:H     | 3        | 0.11          |
| (1,695)  | 1:66:A:ASN:H    | 1:69:A:SER:H     | 10       | 0.11          |
| (1,669)  | 1:64:A:LEU:HG   | 1:65:A:VAL:H     | 5        | 0.11          |
| (1,647)  | 1:62:A:GLY:H    | 1:63:A:TYR:HD1   | 19       | 0.11          |
| (1,629)  | 1:60:A:PRO:HA   | 1:62:A:GLY:H     | 4        | 0.11          |
| (1,629)  | 1:60:A:PRO:HA   | 1:62:A:GLY:H     | 10       | 0.11          |
| (1,608)  | 1:58:A:HIS:HA   | 1:65:A:VAL:H     | 8        | 0.11          |
| (1,608)  | 1:58:A:HIS:HA   | 1:65:A:VAL:H     | 18       | 0.11          |
| (1,570)  | 1:55:A:LEU:H    | 1:56:A:TRP:HE1   | 7        | 0.11          |
| (1,570)  | 1:55:A:LEU:H    | 1:56:A:TRP:HE1   | 9        | 0.11          |
| (1,545)  | 1:53:A:SER:HA   | 1:68:A:LYS:H     | 12       | 0.11          |
| (1,488)  | 1:47:A:ARG:HA   | 1:49:A:LYS:H     | 2        | 0.11          |
| (1,488)  | 1:47:A:ARG:HA   | 1:49:A:LYS:H     | 18       | 0.11          |
| (1,484)  | 1:46:A:LEU:HG   | 1:47:A:ARG:H     | 17       | 0.11          |
| (1,483)  | 1:46:A:LEU:HG   | 1:46:A:LEU:H     | 7        | 0.11          |
| (1,483)  | 1:46:A:LEU:HG   | 1:46:A:LEU:H     | 15       | 0.11          |
| (1,468)  | 1:45:A:THR:HB   | 1:46:A:LEU:H     | 17       | 0.11          |
| (1,453)  | 1:43:A:LEU:H    | 1:135:A:GLY:H    | 11       | 0.11          |
| (1,453)  | 1:43:A:LEU:H    | 1:135:A:GLY:H    | 14       | 0.11          |
| (1,363)  | 1:34:A:SER:H    | 1:36:A:GLU:H     | 1        | 0.11          |
| (1,357)  | 1:34:A:SER:HA   | 1:36:A:GLU:H     | 15       | 0.11          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,334)  | 1:31:A:ASP:H     | 1:41:A:ILE:HA   | 7        | 0.11          |
| (1,334)  | 1:31:A:ASP:H     | 1:41:A:ILE:HA   | 8        | 0.11          |
| (1,330)  | 1:31:A:ASP:HA    | 1:32:A:ASN:H    | 8        | 0.11          |
| (1,330)  | 1:31:A:ASP:HA    | 1:32:A:ASN:H    | 18       | 0.11          |
| (1,330)  | 1:31:A:ASP:HA    | 1:32:A:ASN:H    | 20       | 0.11          |
| (1,291)  | 1:29:A:MET:HA    | 1:56:A:TRP:HE1  | 10       | 0.11          |
| (1,286)  | 1:28:A:LEU:HG    | 1:56:A:TRP:HE1  | 13       | 0.11          |
| (1,285)  | 1:28:A:LEU:HG    | 1:29:A:MET:H    | 11       | 0.11          |
| (1,242)  | 1:26:A:TYR:HA    | 1:46:A:LEU:H    | 5        | 0.11          |
| (1,242)  | 1:26:A:TYR:HA    | 1:46:A:LEU:H    | 9        | 0.11          |
| (1,225)  | 1:23:A:SER:H     | 1:25:A:GLY:H    | 7        | 0.11          |
| (1,223)  | 1:23:A:SER:H     | 1:152:A:GLU:H   | 5        | 0.11          |
| (1,214)  | 1:23:A:SER:HA    | 1:24:A:ASN:H    | 1        | 0.11          |
| (1,214)  | 1:23:A:SER:HA    | 1:24:A:ASN:H    | 2        | 0.11          |
| (1,214)  | 1:23:A:SER:HA    | 1:24:A:ASN:H    | 9        | 0.11          |
| (1,214)  | 1:23:A:SER:HA    | 1:24:A:ASN:H    | 12       | 0.11          |
| (1,214)  | 1:23:A:SER:HA    | 1:24:A:ASN:H    | 16       | 0.11          |
| (1,214)  | 1:23:A:SER:HA    | 1:24:A:ASN:H    | 17       | 0.11          |
| (1,195)  | 1:21:A:ASN:H     | 1:155:A:TRP:HH2 | 2        | 0.11          |
| (1,195)  | 1:21:A:ASN:H     | 1:155:A:TRP:HH2 | 6        | 0.11          |
| (1,130)  | 1:18:A:PHE:H     | 1:158:A:VAL:HB  | 1        | 0.11          |
| (1,130)  | 1:18:A:PHE:H     | 1:158:A:VAL:HB  | 12       | 0.11          |
| (1,130)  | 1:18:A:PHE:H     | 1:158:A:VAL:HB  | 17       | 0.11          |
| (1,115)  | 1:17:A:PHE:H     | 1:56:A:TRP:HA   | 3        | 0.11          |
| (1,98)   | 1:16:A:TRP:HD1   | 1:16:A:TRP:H    | 15       | 0.11          |
| (1,98)   | 1:16:A:TRP:HD1   | 1:16:A:TRP:H    | 20       | 0.11          |
| (1,29)   | 1:6:A:PHE:H      | 1:7:A:GLU:H     | 12       | 0.11          |
| (1,1639) | 1:115:A:LEU:HD11 | 1:118:A:LYS:HB2 | 11       | 0.1           |
| (1,1639) | 1:115:A:LEU:HD11 | 1:118:A:LYS:HB3 | 11       | 0.1           |
| (1,1639) | 1:115:A:LEU:HD12 | 1:118:A:LYS:HB2 | 11       | 0.1           |
| (1,1639) | 1:115:A:LEU:HD12 | 1:118:A:LYS:HB3 | 11       | 0.1           |
| (1,1639) | 1:115:A:LEU:HD13 | 1:118:A:LYS:HB2 | 11       | 0.1           |
| (1,1639) | 1:115:A:LEU:HD13 | 1:118:A:LYS:HB3 | 11       | 0.1           |
| (1,1639) | 1:115:A:LEU:HD21 | 1:118:A:LYS:HB2 | 11       | 0.1           |
| (1,1639) | 1:115:A:LEU:HD21 | 1:118:A:LYS:HB3 | 11       | 0.1           |
| (1,1639) | 1:115:A:LEU:HD22 | 1:118:A:LYS:HB2 | 11       | 0.1           |
| (1,1639) | 1:115:A:LEU:HD22 | 1:118:A:LYS:HB3 | 11       | 0.1           |
| (1,1639) | 1:115:A:LEU:HD23 | 1:118:A:LYS:HB2 | 11       | 0.1           |
| (1,1639) | 1:115:A:LEU:HD23 | 1:118:A:LYS:HB3 | 11       | 0.1           |
| (1,1442) | 1:149:A:ASP:HA   | 1:150:A:ARG:H   | 16       | 0.1           |
| (1,1432) | 1:147:A:HIS:H    | 1:148:A:LEU:H   | 10       | 0.1           |
| (1,1242) | 1:123:A:LEU:HG   | 1:124:A:GLY:H   | 17       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1161) | 1:115:A:LEU:HG  | 1:117:A:ASN:H   | 18       | 0.1           |
| (1,1161) | 1:115:A:LEU:HG  | 1:117:A:ASN:H   | 20       | 0.1           |
| (1,1160) | 1:115:A:LEU:HG  | 1:116:A:ALA:H   | 13       | 0.1           |
| (1,1145) | 1:114:A:TYR:HD1 | 1:115:A:LEU:H   | 5        | 0.1           |
| (1,1145) | 1:114:A:TYR:HD1 | 1:115:A:LEU:H   | 6        | 0.1           |
| (1,1145) | 1:114:A:TYR:HD1 | 1:115:A:LEU:H   | 16       | 0.1           |
| (1,998)  | 1:98:A:ASP:HA   | 1:100:A:LEU:H   | 14       | 0.1           |
| (1,940)  | 1:92:A:ALA:HA   | 1:93:A:GLY:H    | 16       | 0.1           |
| (1,864)  | 1:83:A:GLY:H    | 1:139:A:HIS:HD2 | 10       | 0.1           |
| (1,754)  | 1:72:A:VAL:H    | 1:89:A:GLN:H    | 8        | 0.1           |
| (1,702)  | 1:67:A:LYS:HA   | 1:68:A:LYS:H    | 1        | 0.1           |
| (1,702)  | 1:67:A:LYS:HA   | 1:68:A:LYS:H    | 11       | 0.1           |
| (1,702)  | 1:67:A:LYS:HA   | 1:68:A:LYS:H    | 12       | 0.1           |
| (1,702)  | 1:67:A:LYS:HA   | 1:68:A:LYS:H    | 16       | 0.1           |
| (1,702)  | 1:67:A:LYS:HA   | 1:68:A:LYS:H    | 19       | 0.1           |
| (1,702)  | 1:67:A:LYS:HA   | 1:68:A:LYS:H    | 20       | 0.1           |
| (1,695)  | 1:66:A:ASN:H    | 1:69:A:SER:H    | 11       | 0.1           |
| (1,647)  | 1:62:A:GLY:H    | 1:63:A:TYR:HD1  | 9        | 0.1           |
| (1,629)  | 1:60:A:PRO:HA   | 1:62:A:GLY:H    | 7        | 0.1           |
| (1,629)  | 1:60:A:PRO:HA   | 1:62:A:GLY:H    | 12       | 0.1           |
| (1,612)  | 1:58:A:HIS:HD2  | 1:59:A:ASP:H    | 7        | 0.1           |
| (1,603)  | 1:57:A:ARG:H    | 1:65:A:VAL:HB   | 11       | 0.1           |
| (1,570)  | 1:55:A:LEU:H    | 1:56:A:TRP:HE1  | 13       | 0.1           |
| (1,545)  | 1:53:A:SER:HA   | 1:68:A:LYS:H    | 14       | 0.1           |
| (1,505)  | 1:48:A:THR:HB   | 1:48:A:THR:H    | 13       | 0.1           |
| (1,500)  | 1:47:A:ARG:H    | 1:49:A:LYS:H    | 20       | 0.1           |
| (1,488)  | 1:47:A:ARG:HA   | 1:49:A:LYS:H    | 14       | 0.1           |
| (1,488)  | 1:47:A:ARG:HA   | 1:49:A:LYS:H    | 16       | 0.1           |
| (1,453)  | 1:43:A:LEU:H    | 1:135:A:GLY:H   | 9        | 0.1           |
| (1,453)  | 1:43:A:LEU:H    | 1:135:A:GLY:H   | 19       | 0.1           |
| (1,330)  | 1:31:A:ASP:HA   | 1:32:A:ASN:H    | 2        | 0.1           |
| (1,291)  | 1:29:A:MET:HA   | 1:56:A:TRP:HE1  | 19       | 0.1           |
| (1,286)  | 1:28:A:LEU:HG   | 1:56:A:TRP:HE1  | 11       | 0.1           |
| (1,285)  | 1:28:A:LEU:HG   | 1:29:A:MET:H    | 4        | 0.1           |
| (1,242)  | 1:26:A:TYR:HA   | 1:46:A:LEU:H    | 7        | 0.1           |
| (1,214)  | 1:23:A:SER:HA   | 1:24:A:ASN:H    | 4        | 0.1           |
| (1,214)  | 1:23:A:SER:HA   | 1:24:A:ASN:H    | 10       | 0.1           |
| (1,195)  | 1:21:A:ASN:H    | 1:155:A:TRP:HH2 | 7        | 0.1           |
| (1,130)  | 1:18:A:PHE:H    | 1:158:A:VAL:HB  | 6        | 0.1           |
| (1,130)  | 1:18:A:PHE:H    | 1:158:A:VAL:HB  | 16       | 0.1           |
| (1,115)  | 1:17:A:PHE:H    | 1:56:A:TRP:HA   | 5        | 0.1           |
| (1,115)  | 1:17:A:PHE:H    | 1:56:A:TRP:HA   | 10       | 0.1           |

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

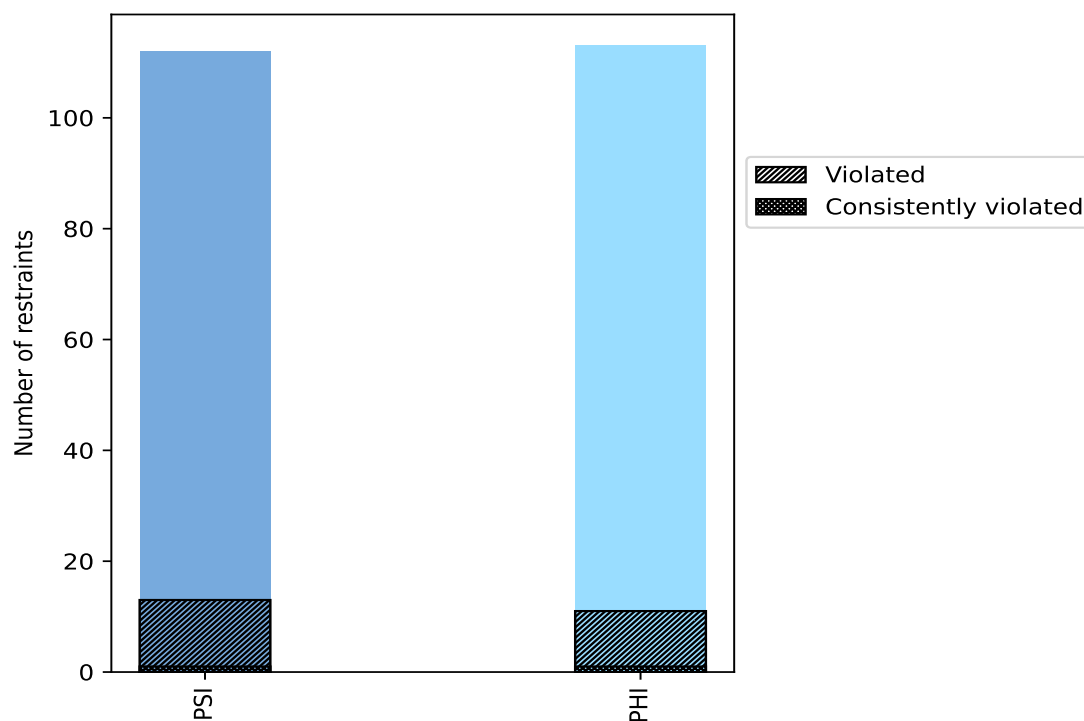
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PSI        | 112   | 49.8           | 13                    | 11.6           | 5.8            | 1                                  | 0.9            | 0.4            |
| PHI        | 113   | 50.2           | 11                    | 9.7            | 4.9            | 1                                  | 0.9            | 0.4            |
| Total      | 225   | 100.0          | 24                    | 10.7           | 10.7           | 2                                  | 0.9            | 0.9            |

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

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



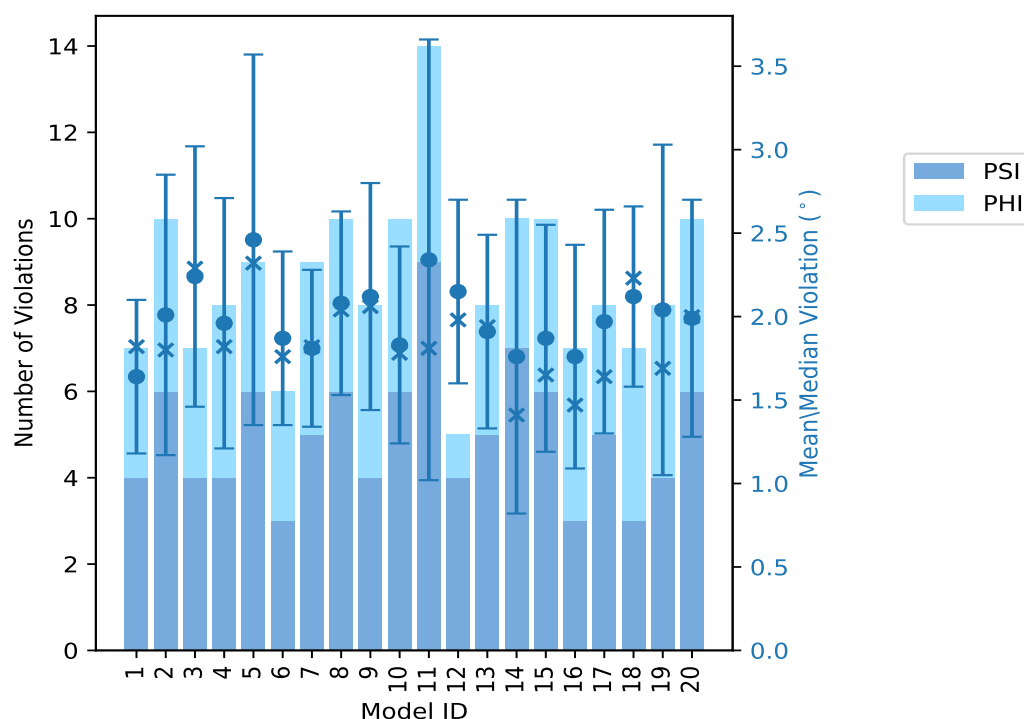
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PSI                  | PHI | Total |          |         |        |            |
| 1        | 4                    | 3   | 7     | 1.64     | 2.17    | 0.46   | 1.82       |
| 2        | 6                    | 4   | 10    | 2.01     | 3.77    | 0.84   | 1.8        |
| 3        | 4                    | 3   | 7     | 2.24     | 3.73    | 0.78   | 2.29       |
| 4        | 4                    | 4   | 8     | 1.96     | 3.5     | 0.75   | 1.82       |
| 5        | 6                    | 3   | 9     | 2.46     | 4.97    | 1.11   | 2.32       |
| 6        | 3                    | 3   | 6     | 1.87     | 2.68    | 0.52   | 1.76       |
| 7        | 5                    | 4   | 9     | 1.81     | 2.62    | 0.47   | 1.82       |
| 8        | 6                    | 4   | 10    | 2.08     | 2.9     | 0.55   | 2.04       |
| 9        | 4                    | 4   | 8     | 2.12     | 3.05    | 0.68   | 2.06       |
| 10       | 6                    | 4   | 10    | 1.83     | 2.98    | 0.59   | 1.78       |
| 11       | 9                    | 5   | 14    | 2.34     | 5.49    | 1.32   | 1.81       |
| 12       | 4                    | 1   | 5     | 2.15     | 3.0     | 0.55   | 1.98       |
| 13       | 5                    | 3   | 8     | 1.91     | 2.83    | 0.58   | 1.94       |
| 14       | 7                    | 3   | 10    | 1.76     | 4.49    | 0.94   | 1.41       |
| 15       | 6                    | 4   | 10    | 1.87     | 3.28    | 0.68   | 1.65       |
| 16       | 3                    | 4   | 7     | 1.76     | 3.16    | 0.67   | 1.47       |
| 17       | 5                    | 3   | 8     | 1.97     | 3.25    | 0.67   | 1.64       |
| 18       | 3                    | 4   | 7     | 2.12     | 2.8     | 0.54   | 2.23       |
| 19       | 4                    | 4   | 8     | 2.04     | 4.42    | 0.99   | 1.69       |
| 20       | 6                    | 4   | 10    | 1.99     | 3.22    | 0.71   | 2.0        |

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



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

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

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

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

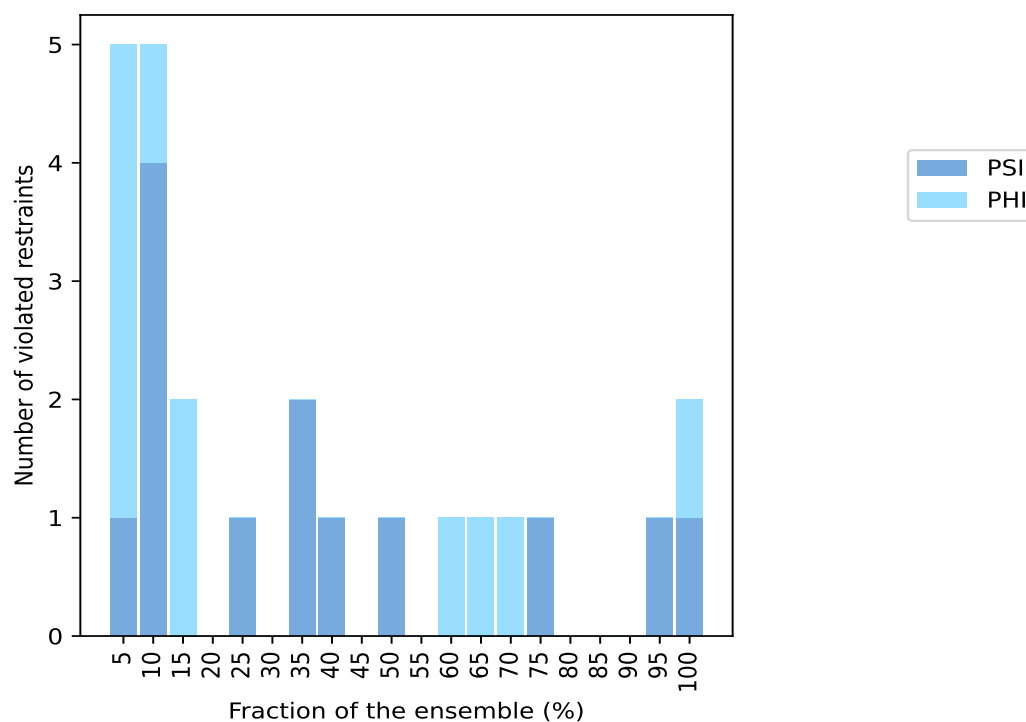
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %     |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

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

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

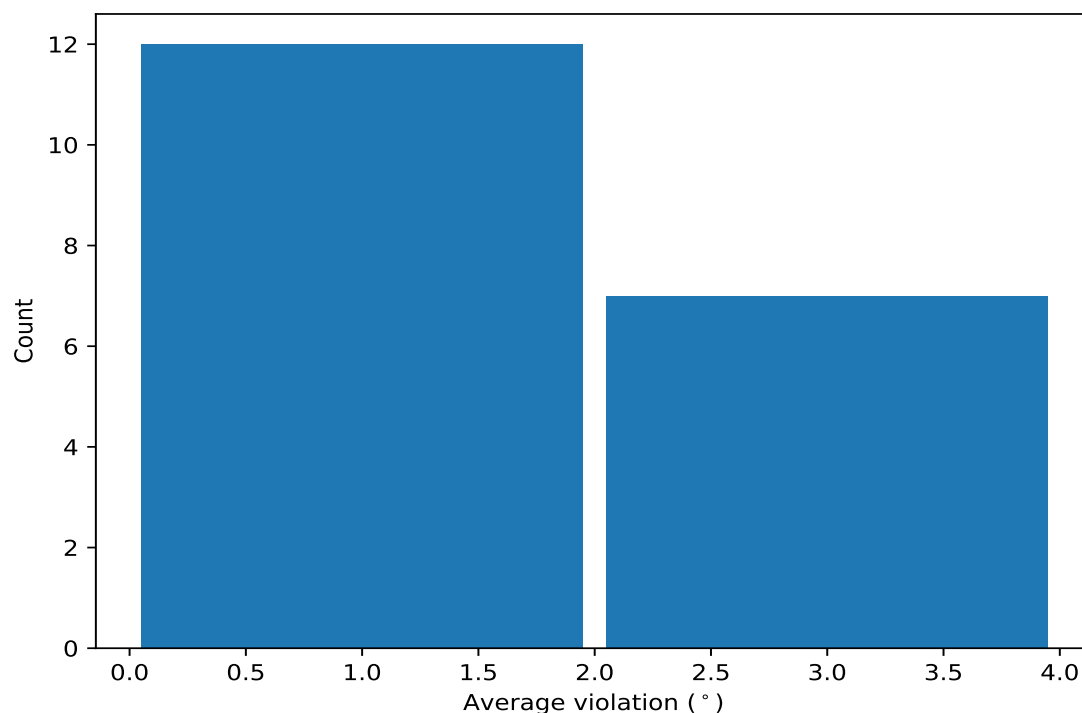


## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

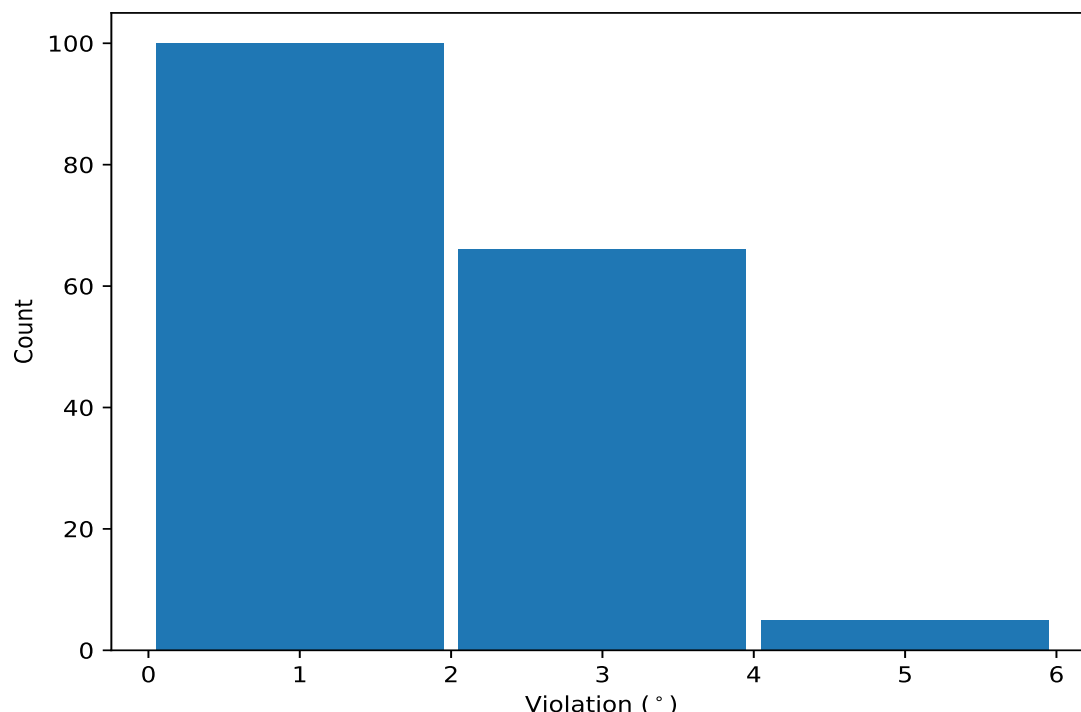
| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,37)  | 1:28:A:LEU:C  | 1:29:A:MET:N   | 1:29:A:MET:CA  | 1:29:A:MET:C  | 20                  | 3.25 | 0.71            | 3.14   |
| (1,169) | 1:121:A:LEU:N | 1:121:A:LEU:CA | 1:121:A:LEU:C  | 1:122:A:ILE:N | 20                  | 2.05 | 0.49            | 2.09   |
| (1,98)  | 1:77:A:LYS:N  | 1:77:A:LYS:CA  | 1:77:A:LYS:C   | 1:78:A:GLY:N  | 19                  | 1.98 | 0.41            | 1.97   |
| (1,205) | 1:148:A:LEU:N | 1:148:A:LEU:CA | 1:148:A:LEU:C  | 1:149:A:ASP:N | 15                  | 1.67 | 0.43            | 1.52   |
| (1,177) | 1:127:A:GLU:C | 1:128:A:SER:N  | 1:128:A:SER:CA | 1:128:A:SER:C | 14                  | 2.14 | 0.41            | 2.04   |
| (1,162) | 1:117:A:ASN:C | 1:118:A:LYS:N  | 1:118:A:LYS:CA | 1:118:A:LYS:C | 13                  | 2.05 | 0.59            | 2.25   |
| (1,128) | 1:98:A:ASP:C  | 1:99:A:ASP:N   | 1:99:A:ASP:CA  | 1:99:A:ASP:C  | 12                  | 1.37 | 0.22            | 1.33   |
| (1,207) | 1:151:A:LYS:N | 1:151:A:LYS:CA | 1:151:A:LYS:C  | 1:152:A:GLU:N | 10                  | 2.16 | 0.57            | 2.41   |
| (1,8)   | 1:10:A:GLU:N  | 1:10:A:GLU:CA  | 1:10:A:GLU:C   | 1:11:A:LYS:N  | 8                   | 1.62 | 0.19            | 1.63   |
| (1,213) | 1:154:A:ARG:N | 1:154:A:ARG:CA | 1:154:A:ARG:C  | 1:155:A:TRP:N | 7                   | 1.77 | 0.51            | 1.62   |
| (1,94)  | 1:75:A:ILE:N  | 1:75:A:ILE:CA  | 1:75:A:ILE:C   | 1:76:A:ALA:N  | 7                   | 1.39 | 0.26            | 1.32   |
| (1,10)  | 1:11:A:LYS:N  | 1:11:A:LYS:CA  | 1:11:A:LYS:C   | 1:12:A:PHE:N  | 5                   | 1.53 | 0.19            | 1.5    |
| (1,134) | 1:101:A:ASN:C | 1:102:A:PHE:N  | 1:102:A:PHE:CA | 1:102:A:PHE:C | 3                   | 1.47 | 0.29            | 1.35   |
| (1,5)   | 1:8:A:LYS:C   | 1:9:A:SER:N    | 1:9:A:SER:CA   | 1:9:A:SER:C   | 3                   | 1.12 | 0.09            | 1.17   |
| (1,119) | 1:91:A:GLN:N  | 1:91:A:GLN:CA  | 1:91:A:GLN:C   | 1:92:A:ALA:N  | 2                   | 3.32 | 2.16            | 3.32   |
| (1,38)  | 1:29:A:MET:N  | 1:29:A:MET:CA  | 1:29:A:MET:C   | 1:30:A:VAL:N  | 2                   | 2.38 | 1.32            | 2.38   |
| (1,122) | 1:95:A:ASN:C  | 1:96:A:VAL:N   | 1:96:A:VAL:CA  | 1:96:A:VAL:C  | 2                   | 1.54 | 0.19            | 1.54   |
| (1,30)  | 1:24:A:ASN:N  | 1:24:A:ASN:CA  | 1:24:A:ASN:C   | 1:25:A:GLY:N  | 2                   | 1.48 | 0.22            | 1.48   |
| (1,133) | 1:101:A:ASN:N | 1:101:A:ASN:CA | 1:101:A:ASN:C  | 1:102:A:PHE:N | 2                   | 1.02 | 0.02            | 1.02   |

<sup>1</sup> Number of violated models, <sup>2</sup>Standard deviation, All angle values are in degree (°)

## 10.5 All violated dihedral-angle restraints [i](#)

### 10.5.1 Histogram : Distribution of violations [i](#)

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



### 10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,119) | 1:91:A:GLN:N | 1:91:A:GLN:CA | 1:91:A:GLN:C  | 1:92:A:ALA:N | 11       | 5.49          |
| (1,118) | 1:90:A:THR:C | 1:91:A:GLN:N  | 1:91:A:GLN:CA | 1:91:A:GLN:C | 11       | 5.05          |
| (1,37)  | 1:28:A:LEU:C | 1:29:A:MET:N  | 1:29:A:MET:CA | 1:29:A:MET:C | 5        | 4.97          |
| (1,37)  | 1:28:A:LEU:C | 1:29:A:MET:N  | 1:29:A:MET:CA | 1:29:A:MET:C | 14       | 4.49          |
| (1,37)  | 1:28:A:LEU:C | 1:29:A:MET:N  | 1:29:A:MET:CA | 1:29:A:MET:C | 19       | 4.42          |
| (1,37)  | 1:28:A:LEU:C | 1:29:A:MET:N  | 1:29:A:MET:CA | 1:29:A:MET:C | 2        | 3.77          |
| (1,37)  | 1:28:A:LEU:C | 1:29:A:MET:N  | 1:29:A:MET:CA | 1:29:A:MET:C | 3        | 3.73          |
| (1,38)  | 1:29:A:MET:N | 1:29:A:MET:CA | 1:29:A:MET:C  | 1:30:A:VAL:N | 5        | 3.7           |
| (1,37)  | 1:28:A:LEU:C | 1:29:A:MET:N  | 1:29:A:MET:CA | 1:29:A:MET:C | 4        | 3.5           |
| (1,37)  | 1:28:A:LEU:C | 1:29:A:MET:N  | 1:29:A:MET:CA | 1:29:A:MET:C | 15       | 3.28          |
| (1,37)  | 1:28:A:LEU:C | 1:29:A:MET:N  | 1:29:A:MET:CA | 1:29:A:MET:C | 17       | 3.25          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,37)  | 1:28:A:LEU:C  | 1:29:A:MET:N   | 1:29:A:MET:CA  | 1:29:A:MET:C  | 20       | 3.22          |
| (1,37)  | 1:28:A:LEU:C  | 1:29:A:MET:N   | 1:29:A:MET:CA  | 1:29:A:MET:C  | 16       | 3.16          |
| (1,37)  | 1:28:A:LEU:C  | 1:29:A:MET:N   | 1:29:A:MET:CA  | 1:29:A:MET:C  | 11       | 3.11          |
| (1,169) | 1:121:A:LEU:N | 1:121:A:LEU:CA | 1:121:A:LEU:C  | 1:122:A:ILE:N | 9        | 3.05          |
| (1,37)  | 1:28:A:LEU:C  | 1:29:A:MET:N   | 1:29:A:MET:CA  | 1:29:A:MET:C  | 12       | 3.0           |
| (1,37)  | 1:28:A:LEU:C  | 1:29:A:MET:N   | 1:29:A:MET:CA  | 1:29:A:MET:C  | 10       | 2.98          |
| (1,162) | 1:117:A:ASN:C | 1:118:A:LYS:N  | 1:118:A:LYS:CA | 1:118:A:LYS:C | 9        | 2.95          |
| (1,207) | 1:151:A:LYS:N | 1:151:A:LYS:CA | 1:151:A:LYS:C  | 1:152:A:GLU:N | 8        | 2.9           |
| (1,177) | 1:127:A:GLU:C | 1:128:A:SER:N  | 1:128:A:SER:CA | 1:128:A:SER:C | 17       | 2.9           |
| (1,37)  | 1:28:A:LEU:C  | 1:29:A:MET:N   | 1:29:A:MET:CA  | 1:29:A:MET:C  | 8        | 2.86          |
| (1,37)  | 1:28:A:LEU:C  | 1:29:A:MET:N   | 1:29:A:MET:CA  | 1:29:A:MET:C  | 13       | 2.83          |
| (1,37)  | 1:28:A:LEU:C  | 1:29:A:MET:N   | 1:29:A:MET:CA  | 1:29:A:MET:C  | 18       | 2.8           |
| (1,207) | 1:151:A:LYS:N | 1:151:A:LYS:CA | 1:151:A:LYS:C  | 1:152:A:GLU:N | 20       | 2.77          |
| (1,98)  | 1:77:A:LYS:N  | 1:77:A:LYS:CA  | 1:77:A:LYS:C   | 1:78:A:GLY:N  | 2        | 2.77          |
| (1,169) | 1:121:A:LEU:N | 1:121:A:LEU:CA | 1:121:A:LEU:C  | 1:122:A:ILE:N | 2        | 2.75          |
| (1,37)  | 1:28:A:LEU:C  | 1:29:A:MET:N   | 1:29:A:MET:CA  | 1:29:A:MET:C  | 9        | 2.72          |
| (1,177) | 1:127:A:GLU:C | 1:128:A:SER:N  | 1:128:A:SER:CA | 1:128:A:SER:C | 3        | 2.68          |
| (1,37)  | 1:28:A:LEU:C  | 1:29:A:MET:N   | 1:29:A:MET:CA  | 1:29:A:MET:C  | 6        | 2.68          |
| (1,162) | 1:117:A:ASN:C | 1:118:A:LYS:N  | 1:118:A:LYS:CA | 1:118:A:LYS:C | 7        | 2.62          |
| (1,162) | 1:117:A:ASN:C | 1:118:A:LYS:N  | 1:118:A:LYS:CA | 1:118:A:LYS:C | 10       | 2.62          |
| (1,213) | 1:154:A:ARG:N | 1:154:A:ARG:CA | 1:154:A:ARG:C  | 1:155:A:TRP:N | 11       | 2.59          |
| (1,98)  | 1:77:A:LYS:N  | 1:77:A:LYS:CA  | 1:77:A:LYS:C   | 1:78:A:GLY:N  | 8        | 2.59          |
| (1,207) | 1:151:A:LYS:N | 1:151:A:LYS:CA | 1:151:A:LYS:C  | 1:152:A:GLU:N | 12       | 2.58          |
| (1,169) | 1:121:A:LEU:N | 1:121:A:LEU:CA | 1:121:A:LEU:C  | 1:122:A:ILE:N | 11       | 2.58          |
| (1,177) | 1:127:A:GLU:C | 1:128:A:SER:N  | 1:128:A:SER:CA | 1:128:A:SER:C | 19       | 2.57          |
| (1,98)  | 1:77:A:LYS:N  | 1:77:A:LYS:CA  | 1:77:A:LYS:C   | 1:78:A:GLY:N  | 20       | 2.52          |
| (1,177) | 1:127:A:GLU:C | 1:128:A:SER:N  | 1:128:A:SER:CA | 1:128:A:SER:C | 15       | 2.5           |
| (1,169) | 1:121:A:LEU:N | 1:121:A:LEU:CA | 1:121:A:LEU:C  | 1:122:A:ILE:N | 4        | 2.5           |
| (1,98)  | 1:77:A:LYS:N  | 1:77:A:LYS:CA  | 1:77:A:LYS:C   | 1:78:A:GLY:N  | 13       | 2.49          |
| (1,207) | 1:151:A:LYS:N | 1:151:A:LYS:CA | 1:151:A:LYS:C  | 1:152:A:GLU:N | 18       | 2.48          |
| (1,205) | 1:148:A:LEU:N | 1:148:A:LEU:CA | 1:148:A:LEU:C  | 1:149:A:ASP:N | 18       | 2.45          |
| (1,207) | 1:151:A:LYS:N | 1:151:A:LYS:CA | 1:151:A:LYS:C  | 1:152:A:GLU:N | 5        | 2.41          |
| (1,207) | 1:151:A:LYS:N | 1:151:A:LYS:CA | 1:151:A:LYS:C  | 1:152:A:GLU:N | 15       | 2.41          |
| (1,162) | 1:117:A:ASN:C | 1:118:A:LYS:N  | 1:118:A:LYS:CA | 1:118:A:LYS:C | 5        | 2.41          |
| (1,177) | 1:127:A:GLU:C | 1:128:A:SER:N  | 1:128:A:SER:CA | 1:128:A:SER:C | 6        | 2.39          |
| (1,205) | 1:148:A:LEU:N | 1:148:A:LEU:CA | 1:148:A:LEU:C  | 1:149:A:ASP:N | 20       | 2.37          |
| (1,169) | 1:121:A:LEU:N | 1:121:A:LEU:CA | 1:121:A:LEU:C  | 1:122:A:ILE:N | 3        | 2.32          |
| (1,169) | 1:121:A:LEU:N | 1:121:A:LEU:CA | 1:121:A:LEU:C  | 1:122:A:ILE:N | 5        | 2.32          |
| (1,213) | 1:154:A:ARG:N | 1:154:A:ARG:CA | 1:154:A:ARG:C  | 1:155:A:TRP:N | 3        | 2.29          |
| (1,169) | 1:121:A:LEU:N | 1:121:A:LEU:CA | 1:121:A:LEU:C  | 1:122:A:ILE:N | 20       | 2.28          |
| (1,162) | 1:117:A:ASN:C | 1:118:A:LYS:N  | 1:118:A:LYS:CA | 1:118:A:LYS:C | 16       | 2.27          |
| (1,162) | 1:117:A:ASN:C | 1:118:A:LYS:N  | 1:118:A:LYS:CA | 1:118:A:LYS:C | 2        | 2.26          |
| (1,98)  | 1:77:A:LYS:N  | 1:77:A:LYS:CA  | 1:77:A:LYS:C   | 1:78:A:GLY:N  | 15       | 2.26          |
| (1,162) | 1:117:A:ASN:C | 1:118:A:LYS:N  | 1:118:A:LYS:CA | 1:118:A:LYS:C | 4        | 2.25          |
| (1,169) | 1:121:A:LEU:N | 1:121:A:LEU:CA | 1:121:A:LEU:C  | 1:122:A:ILE:N | 18       | 2.23          |
| (1,98)  | 1:77:A:LYS:N  | 1:77:A:LYS:CA  | 1:77:A:LYS:C   | 1:78:A:GLY:N  | 9        | 2.23          |
| (1,169) | 1:121:A:LEU:N | 1:121:A:LEU:CA | 1:121:A:LEU:C  | 1:122:A:ILE:N | 7        | 2.22          |
| (1,205) | 1:148:A:LEU:N | 1:148:A:LEU:CA | 1:148:A:LEU:C  | 1:149:A:ASP:N | 8        | 2.18          |
| (1,37)  | 1:28:A:LEU:C  | 1:29:A:MET:N   | 1:29:A:MET:CA  | 1:29:A:MET:C  | 1        | 2.17          |
| (1,162) | 1:117:A:ASN:C | 1:118:A:LYS:N  | 1:118:A:LYS:CA | 1:118:A:LYS:C | 1        | 2.16          |
| (1,205) | 1:148:A:LEU:N | 1:148:A:LEU:CA | 1:148:A:LEU:C  | 1:149:A:ASP:N | 13       | 2.15          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,98)  | 1:77:A:LYS:N  | 1:77:A:LYS:CA  | 1:77:A:LYS:C   | 1:78:A:GLY:N  | 10       | 2.14          |
| (1,169) | 1:121:A:LEU:N | 1:121:A:LEU:CA | 1:121:A:LEU:C  | 1:122:A:ILE:N | 8        | 2.11          |
| (1,37)  | 1:28:A:LEU:C  | 1:29:A:MET:N   | 1:29:A:MET:CA  | 1:29:A:MET:C  | 7        | 2.11          |
| (1,177) | 1:127:A:GLU:C | 1:128:A:SER:N  | 1:128:A:SER:CA | 1:128:A:SER:C | 18       | 2.1           |
| (1,98)  | 1:77:A:LYS:N  | 1:77:A:LYS:CA  | 1:77:A:LYS:C   | 1:78:A:GLY:N  | 3        | 2.1           |
| (1,177) | 1:127:A:GLU:C | 1:128:A:SER:N  | 1:128:A:SER:CA | 1:128:A:SER:C | 7        | 2.09          |
| (1,169) | 1:121:A:LEU:N | 1:121:A:LEU:CA | 1:121:A:LEU:C  | 1:122:A:ILE:N | 17       | 2.07          |
| (1,169) | 1:121:A:LEU:N | 1:121:A:LEU:CA | 1:121:A:LEU:C  | 1:122:A:ILE:N | 13       | 2.02          |
| (1,177) | 1:127:A:GLU:C | 1:128:A:SER:N  | 1:128:A:SER:CA | 1:128:A:SER:C | 2        | 2.0           |
| (1,177) | 1:127:A:GLU:C | 1:128:A:SER:N  | 1:128:A:SER:CA | 1:128:A:SER:C | 10       | 1.99          |
| (1,213) | 1:154:A:ARG:N | 1:154:A:ARG:CA | 1:154:A:ARG:C  | 1:155:A:TRP:N | 4        | 1.98          |
| (1,169) | 1:121:A:LEU:N | 1:121:A:LEU:CA | 1:121:A:LEU:C  | 1:122:A:ILE:N | 12       | 1.98          |
| (1,177) | 1:127:A:GLU:C | 1:128:A:SER:N  | 1:128:A:SER:CA | 1:128:A:SER:C | 8        | 1.97          |
| (1,98)  | 1:77:A:LYS:N  | 1:77:A:LYS:CA  | 1:77:A:LYS:C   | 1:78:A:GLY:N  | 1        | 1.97          |
| (1,98)  | 1:77:A:LYS:N  | 1:77:A:LYS:CA  | 1:77:A:LYS:C   | 1:78:A:GLY:N  | 14       | 1.97          |
| (1,162) | 1:117:A:ASN:C | 1:118:A:LYS:N  | 1:118:A:LYS:CA | 1:118:A:LYS:C | 19       | 1.96          |
| (1,177) | 1:127:A:GLU:C | 1:128:A:SER:N  | 1:128:A:SER:CA | 1:128:A:SER:C | 11       | 1.92          |
| (1,8)   | 1:10:A:GLU:N  | 1:10:A:GLU:CA  | 1:10:A:GLU:C   | 1:11:A:LYS:N  | 8        | 1.91          |
| (1,177) | 1:127:A:GLU:C | 1:128:A:SER:N  | 1:128:A:SER:CA | 1:128:A:SER:C | 9        | 1.9           |
| (1,207) | 1:151:A:LYS:N | 1:151:A:LYS:CA | 1:151:A:LYS:C  | 1:152:A:GLU:N | 13       | 1.87          |
| (1,205) | 1:148:A:LEU:N | 1:148:A:LEU:CA | 1:148:A:LEU:C  | 1:149:A:ASP:N | 6        | 1.87          |
| (1,134) | 1:101:A:ASN:C | 1:102:A:PHE:N  | 1:102:A:PHE:CA | 1:102:A:PHE:C | 11       | 1.87          |
| (1,162) | 1:117:A:ASN:C | 1:118:A:LYS:N  | 1:118:A:LYS:CA | 1:118:A:LYS:C | 8        | 1.85          |
| (1,169) | 1:121:A:LEU:N | 1:121:A:LEU:CA | 1:121:A:LEU:C  | 1:122:A:ILE:N | 1        | 1.82          |
| (1,98)  | 1:77:A:LYS:N  | 1:77:A:LYS:CA  | 1:77:A:LYS:C   | 1:78:A:GLY:N  | 5        | 1.82          |
| (1,10)  | 1:11:A:LYS:N  | 1:11:A:LYS:CA  | 1:11:A:LYS:C   | 1:12:A:PHE:N  | 7        | 1.82          |
| (1,8)   | 1:10:A:GLU:N  | 1:10:A:GLU:CA  | 1:10:A:GLU:C   | 1:11:A:LYS:N  | 10       | 1.8           |
| (1,128) | 1:98:A:ASP:C  | 1:99:A:ASP:N   | 1:99:A:ASP:CA  | 1:99:A:ASP:C  | 13       | 1.78          |
| (1,169) | 1:121:A:LEU:N | 1:121:A:LEU:CA | 1:121:A:LEU:C  | 1:122:A:ILE:N | 10       | 1.75          |
| (1,98)  | 1:77:A:LYS:N  | 1:77:A:LYS:CA  | 1:77:A:LYS:C   | 1:78:A:GLY:N  | 17       | 1.75          |
| (1,94)  | 1:75:A:ILE:N  | 1:75:A:ILE:CA  | 1:75:A:ILE:C   | 1:76:A:ALA:N  | 11       | 1.75          |
| (1,122) | 1:95:A:ASN:C  | 1:96:A:VAL:N   | 1:96:A:VAL:CA  | 1:96:A:VAL:C  | 18       | 1.74          |
| (1,98)  | 1:77:A:LYS:N  | 1:77:A:LYS:CA  | 1:77:A:LYS:C   | 1:78:A:GLY:N  | 11       | 1.74          |
| (1,8)   | 1:10:A:GLU:N  | 1:10:A:GLU:CA  | 1:10:A:GLU:C   | 1:11:A:LYS:N  | 19       | 1.74          |
| (1,8)   | 1:10:A:GLU:N  | 1:10:A:GLU:CA  | 1:10:A:GLU:C   | 1:11:A:LYS:N  | 20       | 1.73          |
| (1,98)  | 1:77:A:LYS:N  | 1:77:A:LYS:CA  | 1:77:A:LYS:C   | 1:78:A:GLY:N  | 16       | 1.71          |
| (1,205) | 1:148:A:LEU:N | 1:148:A:LEU:CA | 1:148:A:LEU:C  | 1:149:A:ASP:N | 5        | 1.7           |
| (1,30)  | 1:24:A:ASN:N  | 1:24:A:ASN:CA  | 1:24:A:ASN:C   | 1:25:A:GLY:N  | 14       | 1.7           |
| (1,10)  | 1:11:A:LYS:N  | 1:11:A:LYS:CA  | 1:11:A:LYS:C   | 1:12:A:PHE:N  | 12       | 1.67          |
| (1,128) | 1:98:A:ASP:C  | 1:99:A:ASP:N   | 1:99:A:ASP:CA  | 1:99:A:ASP:C  | 15       | 1.66          |
| (1,94)  | 1:75:A:ILE:N  | 1:75:A:ILE:CA  | 1:75:A:ILE:C   | 1:76:A:ALA:N  | 4        | 1.66          |
| (1,205) | 1:148:A:LEU:N | 1:148:A:LEU:CA | 1:148:A:LEU:C  | 1:149:A:ASP:N | 19       | 1.65          |
| (1,169) | 1:121:A:LEU:N | 1:121:A:LEU:CA | 1:121:A:LEU:C  | 1:122:A:ILE:N | 6        | 1.65          |
| (1,169) | 1:121:A:LEU:N | 1:121:A:LEU:CA | 1:121:A:LEU:C  | 1:122:A:ILE:N | 15       | 1.65          |
| (1,128) | 1:98:A:ASP:C  | 1:99:A:ASP:N   | 1:99:A:ASP:CA  | 1:99:A:ASP:C  | 19       | 1.63          |
| (1,213) | 1:154:A:ARG:N | 1:154:A:ARG:CA | 1:154:A:ARG:C  | 1:155:A:TRP:N | 14       | 1.62          |
| (1,98)  | 1:77:A:LYS:N  | 1:77:A:LYS:CA  | 1:77:A:LYS:C   | 1:78:A:GLY:N  | 7        | 1.62          |
| (1,98)  | 1:77:A:LYS:N  | 1:77:A:LYS:CA  | 1:77:A:LYS:C   | 1:78:A:GLY:N  | 4        | 1.6           |
| (1,94)  | 1:75:A:ILE:N  | 1:75:A:ILE:CA  | 1:75:A:ILE:C   | 1:76:A:ALA:N  | 2        | 1.59          |
| (1,177) | 1:127:A:GLU:C | 1:128:A:SER:N  | 1:128:A:SER:CA | 1:128:A:SER:C | 20       | 1.56          |
| (1,98)  | 1:77:A:LYS:N  | 1:77:A:LYS:CA  | 1:77:A:LYS:C   | 1:78:A:GLY:N  | 12       | 1.54          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,8)   | 1:10:A:GLU:N  | 1:10:A:GLU:CA  | 1:10:A:GLU:C   | 1:11:A:LYS:N  | 17       | 1.53          |
| (1,207) | 1:151:A:LYS:N | 1:151:A:LYS:CA | 1:151:A:LYS:C  | 1:152:A:GLU:N | 17       | 1.52          |
| (1,205) | 1:148:A:LEU:N | 1:148:A:LEU:CA | 1:148:A:LEU:C  | 1:149:A:ASP:N | 9        | 1.52          |
| (1,205) | 1:148:A:LEU:N | 1:148:A:LEU:CA | 1:148:A:LEU:C  | 1:149:A:ASP:N | 11       | 1.51          |
| (1,10)  | 1:11:A:LYS:N  | 1:11:A:LYS:CA  | 1:11:A:LYS:C   | 1:12:A:PHE:N  | 11       | 1.5           |
| (1,98)  | 1:77:A:LYS:N  | 1:77:A:LYS:CA  | 1:77:A:LYS:C   | 1:78:A:GLY:N  | 6        | 1.49          |
| (1,213) | 1:154:A:ARG:N | 1:154:A:ARG:CA | 1:154:A:ARG:C  | 1:155:A:TRP:N | 2        | 1.48          |
| (1,207) | 1:151:A:LYS:N | 1:151:A:LYS:CA | 1:151:A:LYS:C  | 1:152:A:GLU:N | 16       | 1.47          |
| (1,8)   | 1:10:A:GLU:N  | 1:10:A:GLU:CA  | 1:10:A:GLU:C   | 1:11:A:LYS:N  | 14       | 1.47          |
| (1,128) | 1:98:A:ASP:C  | 1:99:A:ASP:N   | 1:99:A:ASP:CA  | 1:99:A:ASP:C  | 5        | 1.46          |
| (1,8)   | 1:10:A:GLU:N  | 1:10:A:GLU:CA  | 1:10:A:GLU:C   | 1:11:A:LYS:N  | 11       | 1.46          |
| (1,58)  | 1:51:A:TYR:N  | 1:51:A:TYR:CA  | 1:51:A:TYR:C   | 1:52:A:ALA:N  | 15       | 1.44          |
| (1,205) | 1:148:A:LEU:N | 1:148:A:LEU:CA | 1:148:A:LEU:C  | 1:149:A:ASP:N | 17       | 1.41          |
| (1,213) | 1:154:A:ARG:N | 1:154:A:ARG:CA | 1:154:A:ARG:C  | 1:155:A:TRP:N | 7        | 1.39          |
| (1,10)  | 1:11:A:LYS:N  | 1:11:A:LYS:CA  | 1:11:A:LYS:C   | 1:12:A:PHE:N  | 5        | 1.39          |
| (1,205) | 1:148:A:LEU:N | 1:148:A:LEU:CA | 1:148:A:LEU:C  | 1:149:A:ASP:N | 10       | 1.38          |
| (1,205) | 1:148:A:LEU:N | 1:148:A:LEU:CA | 1:148:A:LEU:C  | 1:149:A:ASP:N | 15       | 1.36          |
| (1,128) | 1:98:A:ASP:C  | 1:99:A:ASP:N   | 1:99:A:ASP:CA  | 1:99:A:ASP:C  | 10       | 1.36          |
| (1,128) | 1:98:A:ASP:C  | 1:99:A:ASP:N   | 1:99:A:ASP:CA  | 1:99:A:ASP:C  | 17       | 1.36          |
| (1,177) | 1:127:A:GLU:C | 1:128:A:SER:N  | 1:128:A:SER:CA | 1:128:A:SER:C | 14       | 1.35          |
| (1,134) | 1:101:A:ASN:C | 1:102:A:PHE:N  | 1:102:A:PHE:CA | 1:102:A:PHE:C | 7        | 1.35          |
| (1,122) | 1:95:A:ASN:C  | 1:96:A:VAL:N   | 1:96:A:VAL:CA  | 1:96:A:VAL:C  | 16       | 1.35          |
| (1,8)   | 1:10:A:GLU:N  | 1:10:A:GLU:CA  | 1:10:A:GLU:C   | 1:11:A:LYS:N  | 9        | 1.34          |
| (1,169) | 1:121:A:LEU:N | 1:121:A:LEU:CA | 1:121:A:LEU:C  | 1:122:A:ILE:N | 14       | 1.32          |
| (1,94)  | 1:75:A:ILE:N  | 1:75:A:ILE:CA  | 1:75:A:ILE:C   | 1:76:A:ALA:N  | 14       | 1.32          |
| (1,205) | 1:148:A:LEU:N | 1:148:A:LEU:CA | 1:148:A:LEU:C  | 1:149:A:ASP:N | 3        | 1.3           |
| (1,128) | 1:98:A:ASP:C  | 1:99:A:ASP:N   | 1:99:A:ASP:CA  | 1:99:A:ASP:C  | 3        | 1.29          |
| (1,10)  | 1:11:A:LYS:N  | 1:11:A:LYS:CA  | 1:11:A:LYS:C   | 1:12:A:PHE:N  | 8        | 1.28          |
| (1,128) | 1:98:A:ASP:C  | 1:99:A:ASP:N   | 1:99:A:ASP:CA  | 1:99:A:ASP:C  | 14       | 1.27          |
| (1,30)  | 1:24:A:ASN:N  | 1:24:A:ASN:CA  | 1:24:A:ASN:C   | 1:25:A:GLY:N  | 10       | 1.26          |
| (1,128) | 1:98:A:ASP:C  | 1:99:A:ASP:N   | 1:99:A:ASP:CA  | 1:99:A:ASP:C  | 9        | 1.25          |
| (1,128) | 1:98:A:ASP:C  | 1:99:A:ASP:N   | 1:99:A:ASP:CA  | 1:99:A:ASP:C  | 2        | 1.23          |
| (1,98)  | 1:77:A:LYS:N  | 1:77:A:LYS:CA  | 1:77:A:LYS:C   | 1:78:A:GLY:N  | 19       | 1.22          |
| (1,169) | 1:121:A:LEU:N | 1:121:A:LEU:CA | 1:121:A:LEU:C  | 1:122:A:ILE:N | 16       | 1.21          |
| (1,134) | 1:101:A:ASN:C | 1:102:A:PHE:N  | 1:102:A:PHE:CA | 1:102:A:PHE:C | 8        | 1.2           |
| (1,94)  | 1:75:A:ILE:N  | 1:75:A:ILE:CA  | 1:75:A:ILE:C   | 1:76:A:ALA:N  | 1        | 1.2           |
| (1,5)   | 1:8:A:LYS:C   | 1:9:A:SER:N    | 1:9:A:SER:CA   | 1:9:A:SER:C   | 20       | 1.19          |
| (1,126) | 1:97:A:LYS:C  | 1:98:A:ASP:N   | 1:98:A:ASP:CA  | 1:98:A:ASP:C  | 16       | 1.18          |
| (1,5)   | 1:8:A:LYS:C   | 1:9:A:SER:N    | 1:9:A:SER:CA   | 1:9:A:SER:C   | 11       | 1.17          |
| (1,207) | 1:151:A:LYS:N | 1:151:A:LYS:CA | 1:151:A:LYS:C  | 1:152:A:GLU:N | 2        | 1.16          |
| (1,162) | 1:117:A:ASN:C | 1:118:A:LYS:N  | 1:118:A:LYS:CA | 1:118:A:LYS:C | 6        | 1.16          |
| (1,119) | 1:91:A:GLN:N  | 1:91:A:GLN:CA  | 1:91:A:GLN:C   | 1:92:A:ALA:N  | 20       | 1.16          |
| (1,198) | 1:142:A:LEU:C | 1:143:A:VAL:N  | 1:143:A:VAL:CA | 1:143:A:VAL:C | 4        | 1.15          |
| (1,169) | 1:121:A:LEU:N | 1:121:A:LEU:CA | 1:121:A:LEU:C  | 1:122:A:ILE:N | 19       | 1.12          |
| (1,94)  | 1:75:A:ILE:N  | 1:75:A:ILE:CA  | 1:75:A:ILE:C   | 1:76:A:ALA:N  | 15       | 1.12          |
| (1,205) | 1:148:A:LEU:N | 1:148:A:LEU:CA | 1:148:A:LEU:C  | 1:149:A:ASP:N | 1        | 1.11          |
| (1,162) | 1:117:A:ASN:C | 1:118:A:LYS:N  | 1:118:A:LYS:CA | 1:118:A:LYS:C | 13       | 1.09          |
| (1,128) | 1:98:A:ASP:C  | 1:99:A:ASP:N   | 1:99:A:ASP:CA  | 1:99:A:ASP:C  | 1        | 1.07          |
| (1,94)  | 1:75:A:ILE:N  | 1:75:A:ILE:CA  | 1:75:A:ILE:C   | 1:76:A:ALA:N  | 7        | 1.07          |
| (1,205) | 1:148:A:LEU:N | 1:148:A:LEU:CA | 1:148:A:LEU:C  | 1:149:A:ASP:N | 2        | 1.06          |
| (1,38)  | 1:29:A:MET:N  | 1:29:A:MET:CA  | 1:29:A:MET:C   | 1:30:A:VAL:N  | 14       | 1.06          |

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*Continued from previous page...*

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,11)  | 1:11:A:LYS:C  | 1:12:A:PHE:N   | 1:12:A:PHE:CA  | 1:12:A:PHE:C  | 20       | 1.06          |
| (1,133) | 1:101:A:ASN:N | 1:101:A:ASN:CA | 1:101:A:ASN:C  | 1:102:A:PHE:N | 13       | 1.04          |
| (1,213) | 1:154:A:ARG:N | 1:154:A:ARG:CA | 1:154:A:ARG:C  | 1:155:A:TRP:N | 10       | 1.03          |
| (1,128) | 1:98:A:ASP:C  | 1:99:A:ASP:N   | 1:99:A:ASP:CA  | 1:99:A:ASP:C  | 4        | 1.03          |
| (1,162) | 1:117:A:ASN:C | 1:118:A:LYS:N  | 1:118:A:LYS:CA | 1:118:A:LYS:C | 18       | 1.02          |
| (1,133) | 1:101:A:ASN:N | 1:101:A:ASN:CA | 1:101:A:ASN:C  | 1:102:A:PHE:N | 11       | 1.01          |
| (1,5)   | 1:8:A:LYS:C   | 1:9:A:SER:N    | 1:9:A:SER:CA   | 1:9:A:SER:C   | 15       | 1.0           |